A Low Spin d^5 Iron Imide: Nitrene Capture by Low Coordinate Iron(I) Provides the 4-Coordinate Fe(III) Complex $[PhB(CH_2PPh_2)_3]Fe{\equiv}N$-*p*-tolyl.

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Supporting Information

I. Experimental Section

All manipulations were carried out using standard Schlenk or glove-box techniques under a dinitrogen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thorough sparging with N_2 gas followed by passage through an activated alumina column. Non-halogenated solvents were tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. [Tl][$PhBP_3$][1] and *p*-tolylazide[2] were prepared according to literature procedures. Elemental analyses were performed by Desert Analytics, Tucson, AZ. Deuterated benzene was purchased from Cambridge Isotope Laboratories, Inc. and was degassed and dried over activated 3 Å molecular sieves prior to use. A Varian Mercury-300 NMR spectrometer was used to record ^{1}H NMR spectra at ambient temperature. ^{1}H chemical shifts were referenced to residual solvent. MS data for samples were obtained by injecting a benzene solution into a Hewlett-Packard 1100MSD mass spectrometer equipped with an electrospray (ES) ionization chamber. UV-vis measurements were taken on a Hewlett Packard 8452A Diode Array Spectrometer using a quartz cell with a Teflon cap. IR measurements were obtained with a KBr solution cell using a Bio-Rad Excalibur FTS 3000 spectrometer controlled by Bio-Rad Merlin Software (v. 2.97) set at 4 cm^{-1} resolution. X-ray diffraction studies were carried out in the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer.

Magnetic Measurements. Measurements were recorded using a Quantum Designs SQUID magnetometer running MPMSR2 software (Magnetic Property Measurement System Revision 2). Data were recorded at 5000 G. Samples were suspended in the magnetometer in a clear plastic straw sealed under nitrogen with Lilly No. 4 gel caps. Loaded samples were centered within the magnetometer using the DC centering scan at 35 K and 5000 G. Data were acquired at 2 – 10 K (one data point every 2 K), 10 – 60 K (one data point every 5 K), and 60 – 310 K (one data point every 10 K). The magnetic susceptibility was adjusted for diamagnetic contributions using the constitutive corrections of Pascal's constants. The molar magnetic susceptibility (χ_m) was calculated by converting the calculated magnetic susceptibility (χ) obtained from the magnetometer to a molar susceptibility (using the multiplication factor {(molecular weight)/[sample weight)*(field strength)]}). Curie-Weiss behavior was verified by a plot of χ_m^{-1} versus T. Effective magnetic moments were calculated using Equation 1. Solution magnetic moments were measured using Evans method.[3]

$$\mu_{eff} = \text{sqrt}(7.997\ \chi_m T) \quad \text{(eqn. 1)}$$

EPR Measurements. X-band EPR spectra were obtained on a Bruker EMX spectrometer (controlled by Bruker Win EPR Software v. 3.0) equipped with a rectangular cavity working in the TE_{102} mode. Variable temperature measurements were conducted with an Oxford continuous-flow helium cryostat (temperature range 3.6 – 300

[1] Shapiro, I. R.; Jenkins, D. M.; Thomas, J. C.; Day, M. W.; Peters, J. C. *Chem. Commun.* **2001,** 2152.
[2] Smith, P. A. S.; Brown, B. B. *J. Am. Chem. Soc.* **1951,** *73,* 2438.
[3] (a) Sur, S. K. *J. Magn. Reson.* **1989,** *82,* 169. (b) Evans, D. F. *J. Chem. Soc.* **1959,** 2003.

K). Accurate frequency values were provided by a frequency counter built into the microwave bridge. Solution spectra were acquired in toluene. Sample preparation was performed under a dinitrogen atmosphere in an EPR tube equipped with a ground glass joint.

Electrochemistry. Electrochemical measurements were carried out in a glove-box under a dinitrogen atmosphere in a one-compartment cell using a BAS model 100/W electrochemical analyzer. A glassy carbon electrode and platinum wire were used as the working and auxiliary electrodes, respectively. The reference electrode was $Ag/AgNO_3$ in THF. Solutions (THF) of electrolyte (0.3 M tetra-*n*-butylammonium hexafluorophosphate) and analyte (2 μM) were also prepared in a glove-box.

Synthesis of [PhBP$_3$]FeCl, 1: $FeCl_2$ (0.285 g, 2.25 mmol) was added to THF (80 mL) with stirring. A THF slurry (40 mL) of [Tl][$PhBP_3$] (2.00 g, 2.25 mmol) was then added dropwise. During the addition, the reaction yellowed as TlCl precipitated from solution. After stirring overnight at room temperature, volatiles were removed *in vacuo* and the crude solids were extracted with benzene (~ 30 mL). The benzene extract was then filtered over celite. Removal of the solvent *in vacuo* followed by washing with petroleum ether (3 x 30 mL) and drying afforded **1** as a yellow powder (1.45 g, 83 %). X-ray quality crystals were grown via vapor diffusion of petroleum ether into a benzene solution. ^{1}H NMR (C_6D_6, 300 MHz): δ 40.8 (s); 19.8 (s); 18.3 (s); 7.01 (s); -12.2 (s); -37.7 (br, s). UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 416 (580). SQUID (solid, average 10 – 310 K): μ_{eff} = 4.95 B.M. Evans Method (C_6D_6): 5.04 B.M. ES-MS: calcd. for $C_{45}H_{41}BClFeP_3$ $(M)^+$ 777 m/z, found $(M - Cl)^+$ 741 m/z. Anal. Calcd. for $C_{45}H_{41}BClFeP_3$: C, 69.57; H, 5.32. Found: C, 69.69; H, 5.21.

Synthesis of [PhBP$_3$]FeBr, 2: $FeBr_2$ (0.0240 g, 0.112 mmol) was added to THF (3 mL) with stirring. A THF slurry (3 mL) of [Tl][$PhBP_3$] (0.100 g, 0.112 mmol) was then added dropwise. During the addition, the reaction changed from brown to yellow as TlBr precipitated from solution. After stirring overnight, volatiles were removed *in vacuo* and the crude solids were extracted with benzene (3 mL), filtered over Celite, lyophilized, and washed with petroleum ether (3 x 5 mL). The resulting yellow powder was dried *in vacuo* to yield **2** (0.0775 g, 84 %). ^{1}H NMR (C_6D_6, 300 MHz): δ 37.0 (s); 18.2 (s); 17.1 (s); 8.89 (s); -11.2 (s); -32.9 (br, s). UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 424 (620). Evans Method (C_6D_6): 5.20 B.M. ES-MS: calcd. for $C_{45}H_{41}BBrFeP_3$ $(M)^+$ 821 m/z, found $(M - Br)^+$ 741 m/z. Anal. Calcd. for $C_{45}H_{41}BBrFeP_3$: C, 65.81; H, 5.03. Found: C, 65.42; H, 4.87.

Synthesis of [PhBP$_3$]FeI, 3: FeI_2 (0.100 g, 0.323 mmol) was added to a THF/Et_2O solution (3 mL/3 mL) with stirring. A THF slurry (3 mL) of [Tl][$PhBP_3$] (0.287 g, 0.323 mmol) was then added dropwise. During the addition, the reaction gradually changed from purple to yellow as TlI precipitated from solution. After stirring overnight, volatiles were removed *in vacuo* and the crude solids were extracted with benzene (5 mL), filtered over Celite, lyophilized, and washed with petroleum ether (3 x 5 mL). The resulting yellow powder was dried *in vacuo* to yield **3** (0.237 g, 85 %). ^{1}H NMR (C_6D_6, 300 MHz): δ 29.4 (s); 15.1 (s); 14.6 (s); 12.1 (s); -8.96 (s); -22.9 (br, s). UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 438 (650). Evans Method (C_6D_6): 5.03 B.M. ES-MS: calcd. for

$C_{45}H_{41}BIFeP_3$ $(M)^+$ 868 m/z, found $(M - I)^+$ 741 m/z. Anal. Calcd. for $C_{45}H_{41}BIFeP_3$: C, 62.25; H, 4.76. Found: C, 62.60; H, 4.72.

Synthesis of [PhBP$_3$]FePPh$_3$, 4: A 0.19 weight % Na/Hg amalgam (0.0296 g, 1.29 mmol of sodium dissolved in 15.6 g of mercury) was stirred in THF (50 mL). To this was added dropwise a THF solution (20 mL) of **1** (1.00 g, 1.29 mmol) and PPh_3 (1.01 g, 3.86 mmol). During the addition, the reaction changed from yellow to orange and finally a brown color approximately 20 minutes after the addition was complete. After 15 hours, the reaction solution was decanted from the mercury and volatiles were removed *in vacuo*. The crude solids were extracted with benzene (50 mL) and filtered over Celite. The filtrate was then concentrated *in vacuo* to approximately 20 mL, at which point a small amount of precipitate was evident. The addition of petroleum ether (150 mL) resulted in the precipitation of orange solids which were collected on a sintered glass frit and washed with petroleum ether (3 x 15 mL). After drying *in vacuo*, **4** was obtained as an orange powder (0.795 g, 62 %). X-ray quality crystals were grown via vapor diffusion of petroleum ether into a benzene solution. ^{1}H NMR (C_6D_6, 300 MHz): δ 13.1 (br, s); 11.1 (br, s); 8.51 (s); 7.49 (s); -1.09 (br, s); -2.68 (br, s). Evans Method (C_6D_6): 3.88 B.M. SQUID (solid, average 10 – 310 K): μ_{eff} = 4.09 B.M. ES-MS: calcd. for $C_{63}H_{56}BFeP_4$ $(M)^+$ 1004 m/z, found $(M - PPh_3)^+$ 741 m/z. Anal. Calcd. for $C_{63}H_{56}BFeP_4$: C, 75.39; H, 5.62. Found: C, 75.60; H, 5.61.

Synthesis of [PhBP$_3$]FeNTol, 5: Compound **4** (0.600 g, 0.598 mmol) was dissolved in benzene (15 mL) with stirring. A benzene solution (2 mL) of *p*-tolylazide (0.159 g, 1.19 mmol) was added dropwise, during which time the reaction changed color from orange to an intense forest green. After 12 hours, volatiles were removed *in vacuo* and the solids were washed with petroleum ether (3 x 20 mL) and collected on a sintered glass frit. Drying in vacuo yielded 0.453 g of a forest green powder contaminated with the Ph_3P=N(*p*-tolyl) by-product. Crystallization from petroleum ether into benzene yielded pure **5** (0.255 g, 50 %). ^{1}H NMR (C_6D_6, 300 MHz): δ 26.4 (br, s); 13.8 (s); 13.3 (s); 10.4 (br, s); 9.90 (t, J = 6.6 Hz); 9.08 (t, J = 6.9 Hz); 7.93 (br, s); 5.47 (d, J = 6.6 Hz); 3.14 (s); -0.75 (s). UV-vis (C_6H_6) λ_{max}, nm (ε, M^{-1} cm^{-1}): 640 (3300). SQUID (solid, average 10 – 310 K): μ_{eff} = 2.03 B.M. Evans Method (C_6D_6): 1.85 B.M. Anal. Calcd. for $C_{52}H_{48}BFeNP_3$: C, 73.78; H, 5.72; N, 1.65. Found: C, 73.62; H, 5.84; N, 1.93.

Synthesis of [PhBP$_3$]Fe(CO)$_2$, 6: A benzene solution (3 mL) of **4** (0.100 g, 0.0996 mmol) was pressurized with an atmosphere of CO. This resulted in a color change from yellow-orange to light brown. After 30 minutes at room temperature, volatiles were removed *in vacuo* and the resulting tan solid was washed with petroleum ether (3 x 5 mL) and dried *in vacuo* to yield **6** (0.0558 g, 70 %). X-ray quality crystals were grown from vapor diffusion of petroleum ether into a benzene solution. ^{1}H NMR (C_6D_6, 300 MHz): δ 8.97 (br, s); 8.39 (br, s); 7.88 (s); 7.67 (s); 7.38 (s); 7.03 (s); 4.71 (br, s). IR (C_6H_6): 1979, 1914 cm^{-1}. ES-MS: calcd. for $C_{47}H_{41}BFeO_2P_3$ $(M)^+$ 797 m/z, found $(M - 2\ CO)^+$ 741 m/z. Evans Method (C_6D_6): 1.73 B.M. Anal. Calcd. for $C_{47}H_{41}BFeO_2P_3$: C, 70.79; H, 5.18. Found: C, 70.46; H, 4.96.

Quantification of *p*-tolylisocyanate: A J. Young tube was charged with **5** (0.0107 g, 0.0126 mmol), hexamethylbenzene (0.0013 g, 0.0080 mmol), and C_6D_6 (~ 0.5 mL) under an atmosphere of N_2. The addition of an additional atmosphere of CO resulted in a color change from green to purple, and finally yellow-brown within minutes. After allowing the reaction proceed at room temperature for 10 minutes, ^{1}H NMR integration versus the internal standard revealed that *p*-tolylisocyanate had been generated in approximately quantitative yield.

Reaction of 6 with *p*-tolylazide: An NMR tube was charged with **6** (0.0100 g, 0.0125 mmol), *p*-tolylazide (0.0033 g, 0.025 mmol), ferrocene (0.0017 g, 0.0091 mmol), and C_6D_6 (~ 0.5 mL). The reaction gradually (hours) turns forest green and after 44 hours at room temperature, integration versus the internal ferrocene reference revealed that *p*-tolylisocyanate had been generated in 80 % yield. The paramagnetic metal containing product was identified as **5**.

Figure 1. Core-labeled drawing of [$PhBP_3$]FeCl, **1**. Hydrogens have been omitted for clarity.

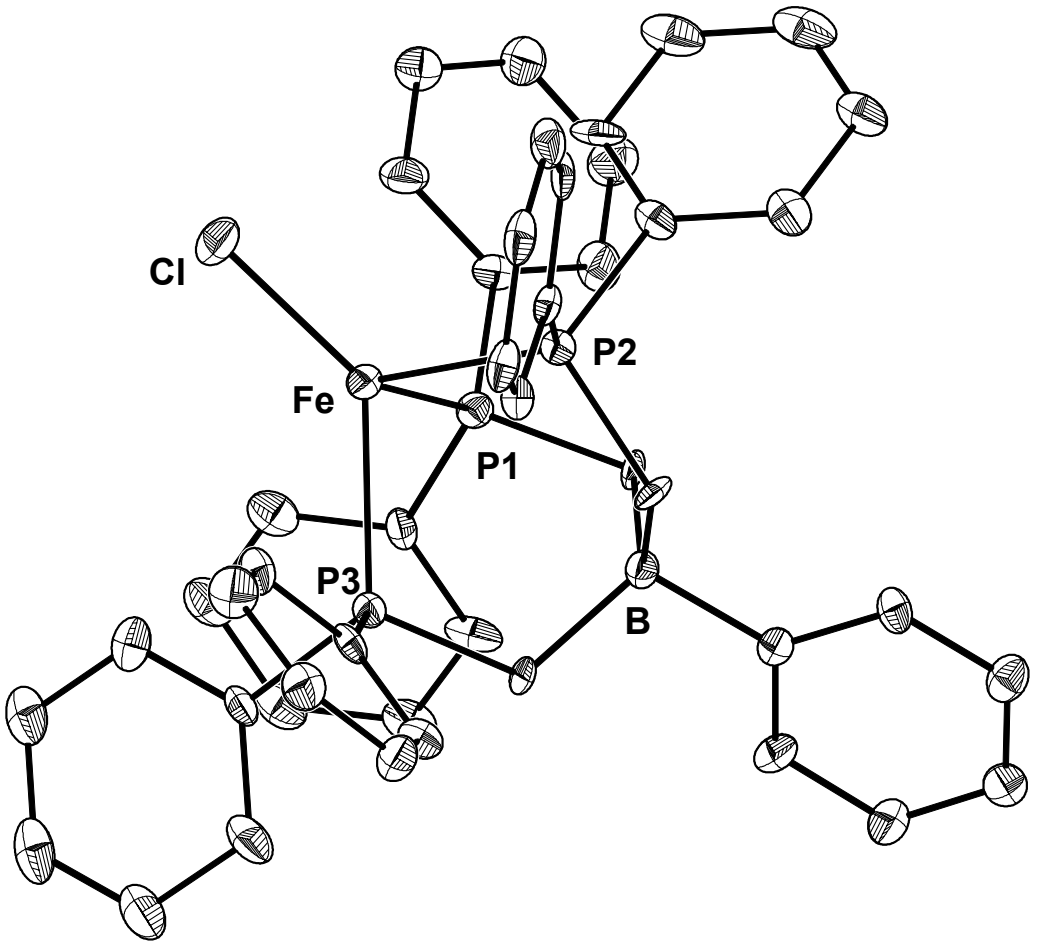

Figure 2. Core-labeled drawing of $[PhBP_3]FePPh_3$, **4**. Hydrogens have been omitted for clarity.

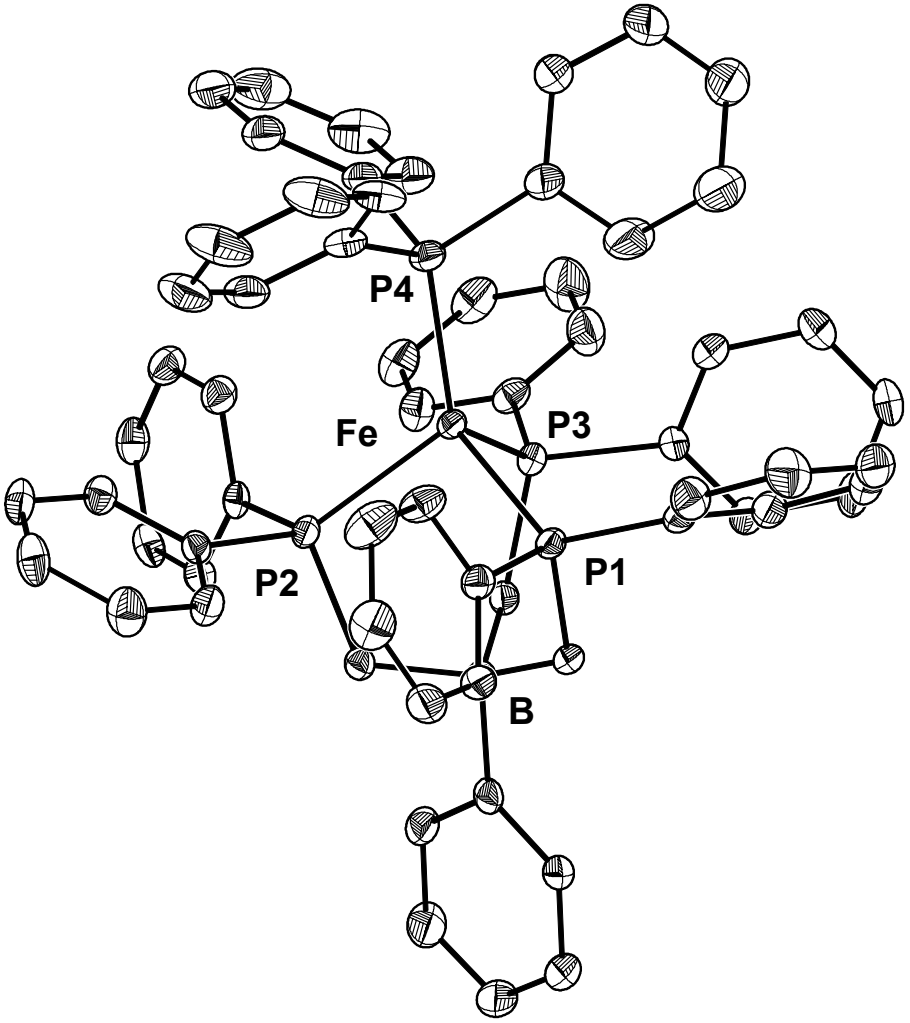

Figure 3. Core-labeled drawing of [$PhBP_3$]FeNTol, **5**. Hydrogens have been omitted for clarity.

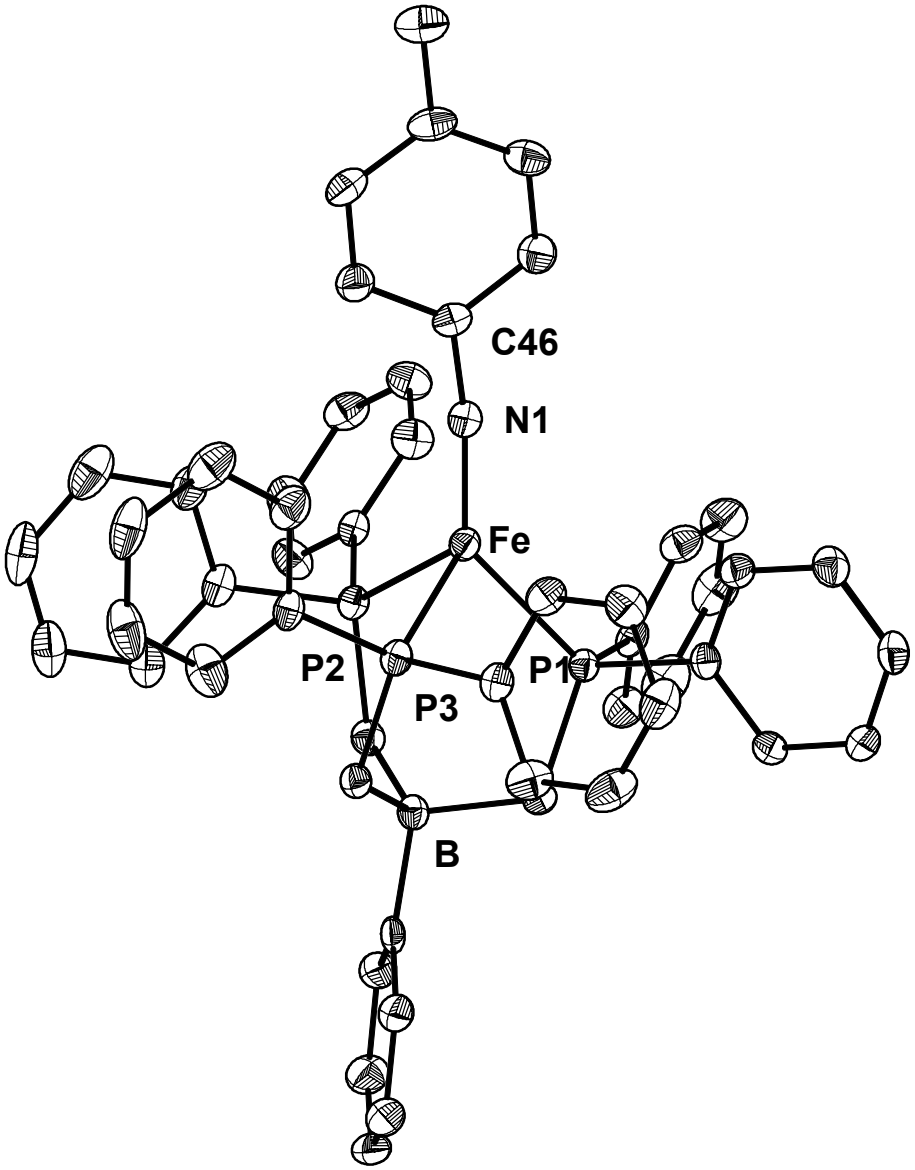

Figure 4. Core-labeled drawing of $[PhBP_3]Fe(CO)_2$, **6**. Hydrogens have been omitted for clarity.

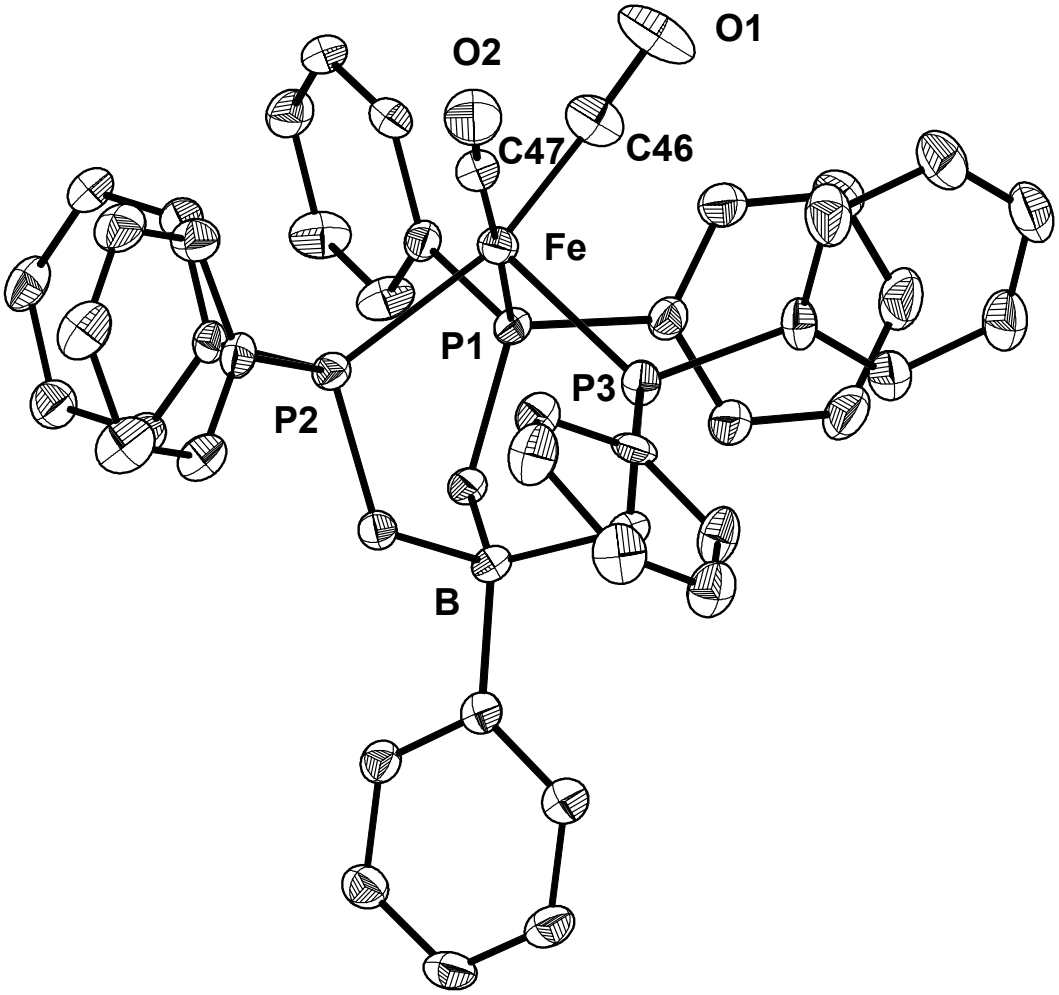

Table 1. Crystal data and structure refinement for $[PhBP_3]FeCl \cdot C_6H_6$.

Identification code	sdb10	
Empirical formula	$C_{51}H_{47}BClFeP_3$	
Formula weight	854.91	
Crystal Habit	block	
Crystal Color	yellow	
Crystal size	0.15 x 0.21 x 0.32 mm^3	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å	
Data collection temperature	96(2) K	
Unit cell dimensions	a = 10.9340(17) Å	α= 90°.
	b = 16.666(3) Å	β= 102.752(13)°.
	c = 24.153(3) Å	γ = 90°.
Volume	4292.8(11) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Density (calculated)	1.323 Mg/m^3	
F(000)	1784	
Theta range for data collection	1.91 to 28.41°.	
Completeness to theta = 28.41°	65.9 %	
Index ranges	-3<=h<=14, -19<=k<=6, -25<=l<=29	
Reflections collected	8120	
Independent reflections	7113 [R(int) = 0.0328]	
Absorption coefficient	0.561 mm^{-1}	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7113 / 0 / 514	
Goodness-of-fit on F^2	1.267	
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.0844	
R indices (all data)	R1 = 0.0670, wR2 = 0.0905	
Largest diff. peak and hole	0.478 and -0.359 $e.Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FeCl \cdot C_6H_6$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe	1453(1)	2477(1)	2195(1)	15(1)
P(1)	1329(1)	3767(1)	2651(1)	15(1)
P(2)	1987(1)	3053(1)	1361(1)	14(1)
P(3)	-784(1)	2535(1)	1790(1)	14(1)
Cl	2654(1)	1432(1)	2495(1)	29(1)
B	-67(3)	4163(2)	1462(2)	14(1)
C(1)	-681(2)	4996(2)	1159(1)	14(1)
C(2)	-218(2)	5429(2)	758(2)	18(1)
C(3)	-735(3)	6150(2)	525(2)	22(1)
C(4)	-1763(2)	6474(2)	696(2)	20(1)
C(5)	-2233(3)	6076(2)	1103(2)	24(1)
C(6)	-1696(3)	5357(2)	1331(2)	21(1)
C(7)	909(2)	4468(2)	2067(1)	14(1)
C(8)	674(2)	3680(2)	1023(1)	15(1)
C(9)	-1222(2)	3567(2)	1580(1)	15(1)
C(10)	99(2)	3825(2)	3059(1)	16(1)
C(11)	-836(2)	4421(2)	2963(2)	19(1)
C(12)	-1741(3)	4428(2)	3288(2)	22(1)
C(13)	-1738(3)	3857(2)	3699(2)	26(1)
C(14)	-813(3)	3270(2)	3801(2)	26(1)
C(15)	99(3)	3254(2)	3477(2)	21(1)
C(16)	2706(2)	4150(2)	3159(1)	15(1)
C(17)	3565(2)	3616(2)	3471(2)	22(1)
C(18)	4614(3)	3896(2)	3853(2)	25(1)
C(19)	4816(3)	4709(2)	3933(2)	27(1)
C(20)	3957(3)	5244(2)	3627(2)	33(1)
C(21)	2914(3)	4968(2)	3239(2)	26(1)
C(22)	3344(2)	3720(2)	1539(2)	17(1)
C(23)	4152(2)	3653(2)	2061(2)	22(1)
C(24)	5180(3)	4166(2)	2216(2)	29(1)
C(25)	5396(3)	4740(2)	1837(2)	28(1)
C(26)	4608(3)	4810(2)	1309(2)	28(1)
C(27)	3577(3)	4303(2)	1152(2)	21(1)
C(28)	2370(2)	2388(2)	820(1)	15(1)
C(29)	3619(3)	2247(2)	792(2)	21(1)
C(30)	3901(3)	1714(2)	395(2)	23(1)
C(31)	2951(3)	1313(2)	21(2)	22(1)
C(32)	1707(3)	1447(2)	49(2)	22(1)
C(33)	1429(3)	1978(2)	441(2)	20(1)
C(34)	-1159(2)	1878(2)	1172(1)	14(1)
C(35)	-2004(3)	2059(2)	666(2)	20(1)
C(36)	-2241(3)	1508(2)	220(2)	26(1)
C(37)	-1659(3)	764(2)	282(2)	26(1)
C(38)	-832(3)	573(2)	787(2)	26(1)
C(39)	-579(3)	1122(2)	1226(2)	22(1)
C(40)	-1848(2)	2161(2)	2215(2)	17(1)
C(41)	-3141(3)	2278(2)	2036(2)	24(1)
C(42)	-3946(3)	1935(2)	2347(2)	29(1)
C(43)	-3474(3)	1493(2)	2828(2)	30(1)
C(44)	-2186(3)	1389(2)	3017(2)	26(1)
C(45)	-1380(3)	1718(2)	2704(2)	19(1)

C(46)	6270(3)	3093(2)	9283(2)	23(1)
C(47)	7319(3)	3567(2)	9487(2)	25(1)
C(48)	7342(3)	4090(2)	9928(2)	26(1)
C(49)	6318(3)	4144(2)	10179(2)	26(1)
C(50)	5266(3)	3663(2)	9980(2)	24(1)
C(51)	5253(3)	3137(2)	9538(2)	24(1)

Table 3. Bond lengths [Å] and angles [°] for $[PhBP_3]FeCl \cdot C_6H_6$.

Fe-Cl	2.2050(9)	C(40)-C(45)	1.391(5)
Fe-P(2)	2.4155(10)	C(41)-C(42)	1.399(4)
Fe-P(3)	2.4267(9)	C(42)-C(43)	1.377(5)
Fe-P(1)	2.4334(9)	C(43)-C(44)	1.392(4)
P(1)-C(7)	1.811(3)	C(44)-C(45)	1.395(4)
P(1)-C(16)	1.834(3)	C(46)-C(51)	1.387(4)
P(1)-C(10)	1.836(3)	C(46)-C(47)	1.390(4)
P(2)-C(8)	1.817(3)	C(47)-C(48)	1.372(5)
P(2)-C(28)	1.833(3)	C(48)-C(49)	1.388(4)
P(2)-C(22)	1.827(3)	C(49)-C(50)	1.397(4)
P(3)-C(34)	1.823(3)	C(50)-C(51)	1.379(5)
P(3)-C(40)	1.824(3)	Cl-Fe-P(2)	110.58(3)
P(3)-C(9)	1.826(3)	Cl-Fe-P(3)	129.68(3)
B-C(1)	1.642(4)	P(2)-Fe-P(3)	93.19(3)
B-C(8)	1.676(5)	Cl-Fe-P(1)	129.59(4)
B-C(9)	1.681(4)	P(2)-Fe-P(1)	94.27(3)
B-C(7)	1.686(5)	P(3)-Fe-P(1)	89.73(3)
C(1)-C(6)	1.403(4)	C(7)-P(1)-C(16)	109.02(14)
C(1)-C(2)	1.391(4)	C(7)-P(1)-C(10)	107.12(13)
C(2)-C(3)	1.392(4)	C(16)-P(1)-C(10)	102.30(14)
C(3)-C(4)	1.389(4)	C(7)-P(1)-Fe	104.26(11)
C(4)-C(5)	1.376(4)	C(16)-P(1)-Fe	119.39(10)
C(5)-C(6)	1.394(4)	C(10)-P(1)-Fe	114.26(9)
C(10)-C(15)	1.388(4)	C(8)-P(2)-C(28)	108.00(14)
C(10)-C(11)	1.407(4)	C(8)-P(2)-C(22)	106.02(13)
C(11)-C(12)	1.392(4)	C(28)-P(2)-C(22)	103.49(13)
C(12)-C(13)	1.375(5)	C(8)-P(2)-Fe	106.91(10)
C(13)-C(14)	1.390(4)	C(28)-P(2)-Fe	119.33(10)
C(14)-C(15)	1.396(4)	C(22)-P(2)-Fe	112.33(12)
C(16)-C(17)	1.389(4)	C(34)-P(3)-C(40)	101.44(14)
C(16)-C(21)	1.389(4)	C(34)-P(3)-C(9)	109.90(14)
C(17)-C(18)	1.386(4)	C(40)-P(3)-C(9)	108.50(13)
C(18)-C(19)	1.378(4)	C(34)-P(3)-Fe	109.32(9)
C(19)-C(20)	1.385(4)	C(40)-P(3)-Fe	118.08(11)
C(20)-C(21)	1.386(4)	C(9)-P(3)-Fe	109.24(9)
C(22)-C(23)	1.375(5)	C(1)-B-C(8)	109.4(3)
C(22)-C(27)	1.410(4)	C(1)-B-C(9)	109.1(2)
C(23)-C(24)	1.397(4)	C(8)-B-C(9)	108.0(2)
C(24)-C(25)	1.380(5)	C(1)-B-C(7)	104.5(2)
C(25)-C(26)	1.378(5)	C(8)-B-C(7)	113.0(2)
C(26)-C(27)	1.392(4)	C(9)-B-C(7)	112.7(3)
C(28)-C(33)	1.395(4)	C(6)-C(1)-C(2)	114.7(3)
C(28)-C(29)	1.401(4)	C(6)-C(1)-B	120.2(3)
C(29)-C(30)	1.391(4)	C(2)-C(1)-B	124.9(2)
C(30)-C(31)	1.389(4)	C(3)-C(2)-C(1)	123.4(3)
C(31)-C(32)	1.395(4)	C(2)-C(3)-C(4)	119.9(3)
C(32)-C(33)	1.378(4)	C(5)-C(4)-C(3)	118.6(3)
C(34)-C(35)	1.393(4)	C(4)-C(5)-C(6)	120.4(3)
C(34)-C(39)	1.405(4)	C(5)-C(6)-C(1)	122.9(3)
C(35)-C(36)	1.394(5)	B-C(7)-P(1)	118.98(19)
C(36)-C(37)	1.387(4)	B-C(8)-P(2)	115.9(2)
C(37)-C(38)	1.386(5)	B-C(9)-P(3)	116.29(18)
C(38)-C(39)	1.382(5)	C(15)-C(10)-C(11)	119.1(3)
C(40)-C(41)	1.397(4)	C(15)-C(10)-P(1)	118.1(2)

C(11)-C(10)-P(1)	122.7(2)	C(31)-C(30)-C(29)	120.5(3)
C(12)-C(11)-C(10)	119.7(3)	C(30)-C(31)-C(32)	119.2(3)
C(13)-C(12)-C(11)	120.8(3)	C(33)-C(32)-C(31)	120.1(3)
C(12)-C(13)-C(14)	120.1(3)	C(32)-C(33)-C(28)	121.5(3)
C(13)-C(14)-C(15)	119.7(3)	C(35)-C(34)-C(39)	118.3(3)
C(10)-C(15)-C(14)	120.6(3)	C(35)-C(34)-P(3)	125.1(2)
C(17)-C(16)-C(21)	118.9(3)	C(39)-C(34)-P(3)	116.6(2)
C(17)-C(16)-P(1)	119.8(2)	C(34)-C(35)-C(36)	120.6(3)
C(21)-C(16)-P(1)	121.3(2)	C(37)-C(36)-C(35)	120.2(3)
C(16)-C(17)-C(18)	120.4(3)	C(36)-C(37)-C(38)	119.7(3)
C(19)-C(18)-C(17)	120.5(3)	C(39)-C(38)-C(37)	120.3(3)
C(18)-C(19)-C(20)	119.3(3)	C(38)-C(39)-C(34)	120.9(3)
C(19)-C(20)-C(21)	120.4(3)	C(41)-C(40)-C(45)	119.6(3)
C(20)-C(21)-C(16)	120.4(3)	C(41)-C(40)-P(3)	120.4(3)
C(23)-C(22)-C(27)	119.4(3)	C(45)-C(40)-P(3)	119.9(2)
C(23)-C(22)-P(2)	119.3(2)	C(40)-C(41)-C(42)	119.4(3)
C(27)-C(22)-P(2)	121.3(3)	C(43)-C(42)-C(41)	120.6(3)
C(22)-C(23)-C(24)	120.8(3)	C(42)-C(43)-C(44)	120.5(3)
C(25)-C(24)-C(23)	119.5(3)	C(45)-C(44)-C(43)	119.2(3)
C(26)-C(25)-C(24)	120.6(3)	C(44)-C(45)-C(40)	120.8(3)
C(25)-C(26)-C(27)	120.4(3)	C(51)-C(46)-C(47)	119.4(3)
C(26)-C(27)-C(22)	119.4(3)	C(48)-C(47)-C(46)	120.6(3)
C(33)-C(28)-C(29)	118.2(3)	C(47)-C(48)-C(49)	120.1(3)
C(33)-C(28)-P(2)	120.8(2)	C(48)-C(49)-C(50)	119.7(3)
C(29)-C(28)-P(2)	120.9(2)	C(51)-C(50)-C(49)	119.8(3)
C(30)-C(29)-C(28)	120.5(3)	C(50)-C(51)-C(46)	120.4(3)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[PhBP_3]FeCl \cdot C_6H_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe	14(1)	14(1)	16(1)	1(1)	2(1)	1(1)
P(1)	15(1)	14(1)	14(1)	0(1)	2(1)	0(1)
P(2)	14(1)	13(1)	15(1)	0(1)	3(1)	-1(1)
P(3)	13(1)	13(1)	14(1)	1(1)	2(1)	-2(1)
Cl	28(1)	24(1)	34(1)	11(1)	7(1)	9(1)
B	14(2)	14(2)	15(3)	3(2)	4(1)	1(1)
C(1)	14(1)	10(2)	16(2)	1(1)	1(1)	-2(1)
C(2)	18(2)	13(2)	24(2)	-3(1)	8(1)	0(1)
C(3)	26(2)	18(2)	21(3)	2(1)	6(1)	-5(1)
C(4)	21(2)	15(2)	20(2)	2(1)	-1(1)	3(1)
C(5)	22(2)	25(2)	26(3)	7(2)	10(1)	9(1)
C(6)	22(2)	23(2)	20(3)	8(2)	10(1)	3(1)
C(7)	16(1)	14(2)	14(2)	3(1)	5(1)	1(1)
C(8)	14(1)	14(2)	16(2)	3(1)	2(1)	2(1)
C(9)	16(1)	13(2)	17(2)	0(1)	3(1)	2(1)
C(10)	16(1)	16(2)	15(2)	-3(1)	4(1)	-3(1)
C(11)	18(2)	19(2)	19(2)	-4(1)	3(1)	-4(1)
C(12)	17(2)	26(2)	24(3)	-7(2)	4(1)	0(1)
C(13)	20(2)	36(2)	25(3)	-9(2)	10(1)	-8(1)
C(14)	31(2)	26(2)	21(3)	5(2)	5(1)	-10(1)
C(15)	21(2)	22(2)	21(2)	-2(1)	3(1)	-1(1)
C(16)	15(1)	20(2)	11(2)	-2(1)	3(1)	-1(1)
C(17)	21(2)	17(2)	28(3)	2(2)	5(1)	-1(1)
C(18)	18(2)	23(2)	31(3)	2(2)	-2(1)	3(1)
C(19)	19(2)	29(2)	27(3)	-1(2)	-5(1)	-4(1)
C(20)	31(2)	16(2)	44(3)	-1(2)	-5(2)	-3(1)
C(21)	22(2)	18(2)	31(3)	3(2)	-6(1)	1(1)
C(22)	14(1)	12(2)	25(3)	-4(1)	7(1)	0(1)
C(23)	14(2)	21(2)	31(3)	-1(2)	6(1)	0(1)
C(24)	17(2)	38(2)	31(3)	-16(2)	3(1)	-5(1)
C(25)	17(2)	22(2)	48(3)	-15(2)	13(2)	-8(1)
C(26)	26(2)	11(2)	51(3)	-2(2)	19(2)	-4(1)
C(27)	19(2)	18(2)	29(3)	-1(2)	10(1)	2(1)
C(28)	17(1)	11(2)	17(2)	3(1)	6(1)	2(1)
C(29)	18(2)	16(2)	29(3)	1(1)	6(1)	-2(1)
C(30)	20(2)	20(2)	31(3)	1(2)	12(1)	5(1)
C(31)	36(2)	13(2)	22(3)	0(1)	15(2)	6(1)
C(32)	27(2)	15(2)	21(3)	-1(1)	2(1)	-1(1)
C(33)	18(2)	21(2)	20(2)	2(2)	6(1)	2(1)
C(34)	17(1)	9(2)	18(2)	-2(1)	7(1)	-5(1)
C(35)	20(2)	15(2)	23(3)	-1(1)	2(1)	2(1)
C(36)	27(2)	23(2)	23(3)	2(2)	-3(1)	2(1)
C(37)	34(2)	16(2)	26(3)	-6(2)	3(2)	-4(1)
C(38)	32(2)	15(2)	29(3)	-2(2)	1(2)	4(1)
C(39)	23(2)	20(2)	21(3)	2(1)	-3(1)	-1(1)
C(40)	19(2)	11(2)	24(3)	-1(1)	9(1)	-3(1)
C(41)	21(2)	21(2)	30(3)	4(2)	8(1)	-1(1)
C(42)	22(2)	26(2)	44(3)	2(2)	15(2)	0(1)
C(43)	40(2)	15(2)	43(3)	-2(2)	28(2)	-5(1)
C(44)	44(2)	15(2)	19(3)	3(1)	11(2)	2(1)
C(45)	23(2)	16(2)	18(2)	-2(1)	3(1)	1(1)
C(46)	31(2)	17(2)	20(3)	0(1)	7(1)	0(1)
C(47)	21(2)	30(2)	25(3)	8(2)	6(1)	2(1)
C(48)	22(2)	25(2)	28(3)	3(2)	-1(1)	-7(1)
C(49)	36(2)	22(2)	17(3)	-1(2)	1(1)	2(1)
C(50)	22(2)	23(2)	28(3)	1(2)	8(1)	4(1)

C(51)	20(2)	14(2)	35(3)	4(2)	2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FeCl{\cdot}C_6H_6$.

	x	y	z	U(eq)
H(2)	488	5222	635	21
H(3)	-385	6421	250	26
H(4)	-2133	6960	535	24
H(5)	-2929	6292	1229	29
H(6)	-2031	5100	1616	25
H(7A)	525	4942	2207	17
H(7B)	1696	4651	1968	17
H(8A)	983	4083	785	18
H(8B)	56	3338	766	18
H(9A)	-1893	3551	1229	18
H(9B)	-1583	3815	1880	18
H(11)	-850	4816	2678	23
H(12)	-2369	4833	3225	27
H(13)	-2369	3863	3914	31
H(14)	-800	2881	4090	31
H(15)	724	2848	3543	26
H(17)	3432	3055	3422	26
H(18)	5199	3526	4062	30
H(19)	5536	4899	4196	32
H(20)	4084	5805	3684	39
H(21)	2337	5340	3027	31
H(23)	4008	3252	2319	26
H(24)	5726	4121	2580	35
H(25)	6095	5090	1941	34
H(26)	4768	5205	1051	33
H(27)	3036	4350	787	26
H(29)	4277	2518	1046	25
H(30)	4751	1623	380	27
H(31)	3147	951	-251	27
H(32)	1050	1172	-203	26
H(33)	578	2067	454	24
H(35)	-2422	2562	623	24
H(36)	-2802	1643	-127	31
H(37)	-1826	388	-21	31
H(38)	-438	61	831	31
H(39)	-4	985	1569	27
H(41)	-3470	2588	1707	28
H(42)	-4826	2009	2225	35
H(43)	-4031	1256	3032	36
H(44)	-1860	1099	3356	31
H(45)	-501	1638	2825	23
H(46)	6250	2741	8972	27
H(47)	8026	3529	9320	30
H(48)	8059	4416	10061	31
H(49)	6332	4506	10484	31
H(50)	4562	3697	10149	29
H(51)	4543	2804	9407	28

Table 6. Crystal data and structure refinement for $[PhBP_3]FePPh_3$ (CCDC 192834).

Empirical formula	$C_{71}H_{69}BP_4Fe$
Formula weight	1112.80
Crystallization Solvent	Petroleum ether/benzene
Crystal Habit	Plate
Crystal size	0.29 x 0.25 x 0.13 mm^3
Crystal color	Pale orange
Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 37660 reflections used in lattice determination	2.28 to 28.42°
Unit cell dimensions	a = 20.2596(6) Å b = 17.7356(6) Å c = 33.4617(11) Å
Volume	12023.3(7) $Å^3$
Z	8
Crystal system	Orthorhombic
Space group	Pbca
Density (calculated)	1.230 Mg/m^3
F(000)	4688
θ range for data collection	1.58 to 28.58°
Completeness to θ = 28.58°	95.8 %
Index ranges	$-26 \le h \le 27$, $-23 \le k \le 23$, $-44 \le l \le 45$
Data collection scan type	ω scans at 5 ϕ settings
Reflections collected	174637
Independent reflections	14706 [R_{int}= 0.0909]
Absorption coefficient	0.399 mm^{-1}
Absorption correction	None
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	14706 / 76 / 711
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	3.208
Final R indices [I>2σ(I), 10408 reflections]	R1 = 0.0713, *w*R2 = 0.1170

R indices (all data)	R1 = 0.1078, *w*R2 = 0.1190
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.196 and -0.559 e.Å^{-3}

Special Refinement Details

The crystal contains solvent of crystallization located in two different disordered sites (per asymmetric unit). For one site (shown in Figure 4), the difference electron density Fourier contains nearly planar electron density distributed over five maxima. During refinement the 1-2 and 1-3 distances between these maxima (modeled as carbon) were restrained to be equal. The 1-2 distances refined to approx 1.50Å, suggesting carbon-carbon single bonds. However, the refined positions were very nearly co-planar. This site was most satisfactorily modeled as cyclopentane (with riding hydrogen atoms). The second site (see Figure 5), near a center of symmetry, shows six maxima in the difference electron density Fourier. With the peaks modeled as carbon (restrained as in the first site), the distances tend towards <1.3Å and the peaks are not as coplanar. Because of the short distances this site was modeled as a rigid benzene (riding hydrogens) at half occupancy to accommodate the nearby center of symmetry.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FePPh_3$ (CCDC 192834). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Fe(1)	5005(1)	8976(1)	1537(1)	17(1)	1
P(1)	5900(1)	8420(1)	1864(1)	19(1)	1
P(2)	4797(1)	9928(1)	2005(1)	17(1)	1
P(3)	4217(1)	8131(1)	1779(1)	18(1)	1
P(4)	5052(1)	9288(1)	874(1)	23(1)	1
B(1)	4905(2)	8566(2)	2532(1)	18(1)	1
C(1)	4904(2)	8415(2)	3012(1)	18(1)	1
C(2)	4564(2)	7835(2)	3206(1)	21(1)	1
C(3)	4592(2)	7724(2)	3617(1)	27(1)	1
C(4)	4959(2)	8192(2)	3852(1)	36(1)	1
C(5)	5308(2)	8778(2)	3670(1)	36(1)	1
C(6)	5275(2)	8885(2)	3262(1)	25(1)	1
C(7)	5700(2)	8504(2)	2395(1)	19(1)	1
C(8)	4603(2)	9430(2)	2466(1)	17(1)	1
C(9)	4434(2)	7927(2)	2297(1)	19(1)	1
C(10)	5959(2)	7416(2)	1739(1)	20(1)	1
C(11)	6048(2)	6843(2)	2020(1)	23(1)	1
C(12)	6114(2)	6103(2)	1898(1)	29(1)	1
C(13)	6105(2)	5926(2)	1499(1)	38(1)	1
C(14)	6016(2)	6490(2)	1213(1)	40(1)	1
C(15)	5934(2)	7232(2)	1337(1)	30(1)	1
C(16)	6783(2)	8664(2)	1833(1)	21(1)	1
C(17)	7010(2)	9341(2)	1997(1)	25(1)	1
C(18)	7663(2)	9546(2)	1979(1)	32(1)	1
C(19)	8119(2)	9077(2)	1796(1)	33(1)	1
C(20)	7902(2)	8403(2)	1630(1)	39(1)	1
C(21)	7244(2)	8206(2)	1645(1)	34(1)	1
C(22)	5546(2)	10492(2)	2100(1)	18(1)	1
C(23)	5760(2)	10701(2)	2477(1)	21(1)	1
C(24)	6331(2)	11112(2)	2525(1)	23(1)	1
C(25)	6700(2)	11331(2)	2195(1)	27(1)	1
C(26)	6489(2)	11142(2)	1817(1)	25(1)	1
C(27)	5922(2)	10717(2)	1769(1)	23(1)	1
C(28)	4163(2)	10668(2)	1970(1)	19(1)	1
C(29)	3502(2)	10507(2)	2037(1)	24(1)	1
C(30)	3023(2)	11050(2)	1986(1)	31(1)	1
C(31)	3193(2)	11774(2)	1863(1)	29(1)	1
C(32)	3844(2)	11947(2)	1796(1)	25(1)	1
C(33)	4327(2)	11401(2)	1847(1)	22(1)	1
C(34)	3409(2)	8582(2)	1777(1)	19(1)	1
C(35)	2925(2)	8476(2)	2065(1)	23(1)	1
C(36)	2308(2)	8802(2)	2028(1)	29(1)	1
C(37)	2166(2)	9242(2)	1702(1)	35(1)	1
C(38)	2647(2)	9355(2)	1408(1)	38(1)	1
C(39)	3256(2)	9029(2)	1446(1)	27(1)	1
C(40)	3997(2)	7218(2)	1551(1)	19(1)	1
C(41)	4428(2)	6606(2)	1585(1)	25(1)	1
C(42)	4291(2)	5928(2)	1393(1)	30(1)	1
C(43)	3719(2)	5848(2)	1171(1)	34(1)	1
C(44)	3287(2)	6443(2)	1137(1)	37(1)	1
C(45)	3425(2)	7131(2)	1325(1)	27(1)	1
C(46)	5091(2)	8509(2)	518(1)	29(1)	1
C(47)	4773(2)	7852(2)	632(1)	54(1)	1

C(48)	4761(3)	7234(2)	374(1)	76(2)	1
C(49)	5062(3)	7279(2)	11(1)	65(2)	1
C(50)	5380(2)	7927(2)	-102(1)	48(1)	1
C(51)	5396(2)	8543(2)	152(1)	34(1)	1
C(52)	4357(2)	9846(2)	691(1)	24(1)	1
C(53)	3950(2)	9618(2)	382(1)	30(1)	1
C(54)	3396(2)	10036(3)	281(1)	42(1)	1
C(55)	3246(2)	10692(3)	489(1)	49(1)	1
C(56)	3648(2)	10927(2)	802(1)	39(1)	1
C(57)	4192(2)	10511(2)	900(1)	30(1)	1
C(58)	5786(2)	9850(2)	767(1)	24(1)	1
C(59)	5768(2)	10600(2)	634(1)	27(1)	1
C(60)	6338(2)	11027(2)	624(1)	39(1)	1
C(61)	6934(2)	10716(3)	745(1)	46(1)	1
C(62)	6958(2)	9973(3)	874(1)	45(1)	1
C(63)	6393(2)	9544(2)	886(1)	33(1)	1
C(71)	7020(6)	2842(7)	148(4)	487(18)	1
C(72)	7072(7)	2346(9)	-216(4)	588(9)	1
C(73)	7728(6)	1965(6)	-225(4)	337(11)	1
C(74)	8080(5)	2198(9)	150(5)	490(20)	1
C(75)	7632(7)	2729(6)	392(3)	233(8)	1
C(77)	8583(5)	9992(6)	-150(3)	119(5)	0.50
C(78)	8386(4)	9621(6)	196(3)	157(8)	0.50
C(79)	8823(6)	9545(5)	514(2)	111(5)	0.50
C(80)	9457(5)	9839(5)	486(3)	114(6)	0.50
C(81)	9654(4)	10210(5)	140(4)	370(20)	0.50
C(82)	9217(6)	10286(5)	-178(3)	280(16)	0.50

Table 8. Bond lengths [Å] and angles [°] for $[PhBP_3]FePPh_3$ (CCDC 192834).

Fe(1)-P(4)	2.2889(9)	C(20)-H(20)	0.9500
Fe(1)-P(3)	2.3341(10)	C(21)-H(21)	0.9500
Fe(1)-P(1)	2.3350(10)	C(22)-C(23)	1.387(4)
Fe(1)-P(2)	2.3400(10)	C(22)-C(27)	1.402(4)
P(1)-C(7)	1.828(3)	C(23)-C(24)	1.377(4)
P(1)-C(10)	1.833(3)	C(23)-H(23)	0.9500
P(1)-C(16)	1.844(3)	C(24)-C(25)	1.386(5)
P(2)-C(8)	1.819(3)	C(24)-H(24)	0.9500
P(2)-C(28)	1.841(3)	C(25)-C(26)	1.377(5)
P(2)-C(22)	1.845(3)	C(25)-H(25)	0.9500
P(3)-C(9)	1.823(3)	C(26)-C(27)	1.383(4)
P(3)-C(34)	1.822(3)	C(26)-H(26)	0.9500
P(3)-C(40)	1.846(3)	C(27)-H(27)	0.9500
P(4)-C(52)	1.826(4)	C(28)-C(29)	1.387(4)
P(4)-C(58)	1.826(4)	C(28)-C(33)	1.404(4)
P(4)-C(46)	1.826(3)	C(29)-C(30)	1.378(4)
B(1)-C(1)	1.630(5)	C(29)-H(29)	0.9500
B(1)-C(8)	1.664(5)	C(30)-C(31)	1.390(5)
B(1)-C(9)	1.677(5)	C(30)-H(30)	0.9500
B(1)-C(7)	1.677(5)	C(31)-C(32)	1.373(5)
C(1)-C(2)	1.397(4)	C(31)-H(31)	0.9500
C(1)-C(6)	1.400(4)	C(32)-C(33)	1.387(4)
C(2)-C(3)	1.391(4)	C(32)-H(32)	0.9500
C(2)-H(2)	0.9500	C(33)-H(33)	0.9500
C(3)-C(4)	1.363(5)	C(34)-C(35)	1.389(4)
C(3)-H(3)	0.9500	C(34)-C(39)	1.396(4)
C(4)-C(5)	1.397(5)	C(35)-C(36)	1.383(5)
C(4)-H(4)	0.9500	C(35)-H(35)	0.9500
C(5)-C(6)	1.380(4)	C(36)-C(37)	1.373(5)
C(5)-H(5)	0.9500	C(36)-H(36)	0.9500
C(6)-H(6)	0.9500	C(37)-C(38)	1.398(5)
C(7)-H(7A)	0.9900	C(37)-H(37)	0.9500
C(7)-H(7B)	0.9900	C(38)-C(39)	1.367(5)
C(8)-H(8A)	0.9900	C(38)-H(38)	0.9500
C(8)-H(8B)	0.9900	C(39)-H(39)	0.9500
C(9)-H(9A)	0.9900	C(40)-C(45)	1.390(5)
C(9)-H(9B)	0.9900	C(40)-C(41)	1.397(4)
C(10)-C(15)	1.386(4)	C(41)-C(42)	1.391(4)
C(10)-C(11)	1.395(4)	C(41)-H(41)	0.9500
C(11)-C(12)	1.381(4)	C(42)-C(43)	1.383(5)
C(11)-H(11)	0.9500	C(42)-H(42)	0.9500
C(12)-C(13)	1.372(5)	C(43)-C(44)	1.377(5)
C(12)-H(12)	0.9500	C(43)-H(43)	0.9500
C(13)-C(14)	1.395(5)	C(44)-C(45)	1.401(5)
C(13)-H(13)	0.9500	C(44)-H(44)	0.9500
C(14)-C(15)	1.390(5)	C(45)-H(45)	0.9500
C(14)-H(14)	0.9500	C(46)-C(51)	1.373(5)
C(15)-H(15)	0.9500	C(46)-C(47)	1.384(5)
C(16)-C(17)	1.396(4)	C(47)-C(48)	1.395(5)
C(16)-C(21)	1.387(5)	C(47)-H(47)	0.9500
C(17)-C(18)	1.374(5)	C(48)-C(49)	1.361(6)
C(17)-H(17)	0.9500	C(48)-H(48)	0.9500
C(18)-C(19)	1.385(5)	C(49)-C(50)	1.373(5)
C(18)-H(18)	0.9500	C(49)-H(49)	0.9500
C(19)-C(20)	1.390(5)	C(50)-C(51)	1.385(5)
C(19)-H(19)	0.9500	C(50)-H(50)	0.9500
C(20)-C(21)	1.378(5)	C(51)-H(51)	0.9500

C(52)-C(53)	1.383(5)	C(7)-P(1)-Fe(1)	104.38(11)
C(52)-C(57)	1.411(5)	C(10)-P(1)-Fe(1)	110.74(12)
C(53)-C(54)	1.388(5)	C(16)-P(1)-Fe(1)	128.89(11)
C(53)-H(53)	0.9500	C(8)-P(2)-C(28)	104.43(15)
C(54)-C(55)	1.388(5)	C(8)-P(2)-C(22)	107.24(15)
C(54)-H(54)	0.9500	C(28)-P(2)-C(22)	101.41(15)
C(55)-C(56)	1.392(5)	C(8)-P(2)-Fe(1)	104.79(10)
C(55)-H(55)	0.9500	C(28)-P(2)-Fe(1)	126.69(11)
C(56)-C(57)	1.365(5)	C(22)-P(2)-Fe(1)	110.97(11)
C(56)-H(56)	0.9500	C(9)-P(3)-C(34)	107.96(16)
C(57)-H(57)	0.9500	C(9)-P(3)-C(40)	106.11(14)
C(58)-C(59)	1.404(4)	C(34)-P(3)-C(40)	99.52(15)
C(58)-C(63)	1.401(5)	C(9)-P(3)-Fe(1)	106.98(11)
C(59)-C(60)	1.381(5)	C(34)-P(3)-Fe(1)	109.32(11)
C(59)-H(59)	0.9500	C(40)-P(3)-Fe(1)	125.84(11)
C(60)-C(61)	1.386(6)	C(52)-P(4)-C(58)	105.45(16)
C(60)-H(60)	0.9500	C(52)-P(4)-C(46)	103.00(17)
C(61)-C(62)	1.390(5)	C(58)-P(4)-C(46)	104.45(17)
C(61)-H(61)	0.9500	C(52)-P(4)-Fe(1)	115.08(11)
C(62)-C(63)	1.376(5)	C(58)-P(4)-Fe(1)	110.81(11)
C(62)-H(62)	0.9500	C(46)-P(4)-Fe(1)	116.87(11)
C(63)-H(63)	0.9500	C(1)-B(1)-C(8)	106.4(3)
C(71)-C(75)	1.498(9)	C(1)-B(1)-C(9)	110.5(3)
C(71)-C(72)	1.507(11)	C(8)-B(1)-C(9)	110.5(3)
C(71)-H(71A)	0.9900	C(1)-B(1)-C(7)	105.0(3)
C(71)-H(71B)	0.9900	C(8)-B(1)-C(7)	112.2(3)
C(72)-C(73)	1.491(10)	C(9)-B(1)-C(7)	112.0(3)
C(72)-H(72A)	0.9900	C(2)-C(1)-C(6)	115.2(3)
C(72)-H(72B)	0.9900	C(2)-C(1)-B(1)	125.4(3)
C(73)-C(74)	1.501(10)	C(6)-C(1)-B(1)	119.4(3)
C(73)-H(73A)	0.9900	C(3)-C(2)-C(1)	122.9(3)
C(73)-H(73B)	0.9900	C(3)-C(2)-H(2)	118.6
C(74)-C(75)	1.539(10)	C(1)-C(2)-H(2)	118.6
C(74)-H(74A)	0.9900	C(4)-C(3)-C(2)	120.5(3)
C(74)-H(74B)	0.9900	C(4)-C(3)-H(3)	119.8
C(75)-H(75A)	0.9900	C(2)-C(3)-H(3)	119.8
C(75)-H(75B)	0.9900	C(3)-C(4)-C(5)	118.5(3)
C(77)-C(78)	1.3900	C(3)-C(4)-H(4)	120.7
C(77)-C(82)	1.3900	C(5)-C(4)-H(4)	120.7
C(77)-H(77)	0.9500	C(6)-C(5)-C(4)	120.6(3)
C(78)-C(79)	1.3900	C(6)-C(5)-H(5)	119.7
C(78)-H(78)	0.9500	C(4)-C(5)-H(5)	119.7
C(79)-C(80)	1.3900	C(5)-C(6)-C(1)	122.4(3)
C(79)-H(79)	0.9500	C(5)-C(6)-H(6)	118.8
C(80)-C(81)	1.3900	C(1)-C(6)-H(6)	118.8
C(80)-H(80)	0.9500	B(1)-C(7)-P(1)	118.9(2)
C(81)-C(82)	1.3900	B(1)-C(7)-H(7A)	107.6
C(81)-C(81)#1	1.84(2)	P(1)-C(7)-H(7A)	107.6
C(81)-H(81)	0.9500	B(1)-C(7)-H(7B)	107.6
C(82)-H(82)	0.9500	P(1)-C(7)-H(7B)	107.6
P(4)-Fe(1)-P(3)	121.30(4)	H(7A)-C(7)-H(7B)	107.0
P(4)-Fe(1)-P(1)	121.60(4)	B(1)-C(8)-P(2)	118.7(2)
P(3)-Fe(1)-P(1)	95.58(3)	B(1)-C(8)-H(8A)	107.6
P(4)-Fe(1)-P(2)	118.79(3)	P(2)-C(8)-H(8A)	107.6
P(3)-Fe(1)-P(2)	96.19(3)	B(1)-C(8)-H(8B)	107.6
P(1)-Fe(1)-P(2)	97.54(3)	P(2)-C(8)-H(8B)	107.6
C(7)-P(1)-C(10)	108.36(15)	H(8A)-C(8)-H(8B)	107.1
C(7)-P(1)-C(16)	104.53(15)	B(1)-C(9)-P(3)	116.6(2)
C(10)-P(1)-C(16)	98.73(16)	B(1)-C(9)-H(9A)	108.1

P(3)-C(9)-H(9A)	108.1	C(29)-C(28)-P(2)	121.1(2)
B(1)-C(9)-H(9B)	108.1	C(33)-C(28)-P(2)	120.9(3)
P(3)-C(9)-H(9B)	108.1	C(30)-C(29)-C(28)	121.1(3)
H(9A)-C(9)-H(9B)	107.3	C(30)-C(29)-H(29)	119.5
C(15)-C(10)-C(11)	119.1(3)	C(28)-C(29)-H(29)	119.5
C(15)-C(10)-P(1)	116.6(3)	C(29)-C(30)-C(31)	120.5(3)
C(11)-C(10)-P(1)	124.3(3)	C(29)-C(30)-H(30)	119.8
C(12)-C(11)-C(10)	120.4(3)	C(31)-C(30)-H(30)	119.8
C(12)-C(11)-H(11)	119.8	C(32)-C(31)-C(30)	119.5(3)
C(10)-C(11)-H(11)	119.8	C(32)-C(31)-H(31)	120.2
C(13)-C(12)-C(11)	120.3(3)	C(30)-C(31)-H(31)	120.2
C(13)-C(12)-H(12)	119.9	C(31)-C(32)-C(33)	120.1(3)
C(11)-C(12)-H(12)	119.9	C(31)-C(32)-H(32)	120.0
C(12)-C(13)-C(14)	120.3(3)	C(33)-C(32)-H(32)	120.0
C(12)-C(13)-H(13)	119.8	C(32)-C(33)-C(28)	121.0(3)
C(14)-C(13)-H(13)	119.8	C(32)-C(33)-H(33)	119.5
C(13)-C(14)-C(15)	119.3(4)	C(28)-C(33)-H(33)	119.5
C(13)-C(14)-H(14)	120.3	C(35)-C(34)-C(39)	118.1(3)
C(15)-C(14)-H(14)	120.3	C(35)-C(34)-P(3)	124.8(3)
C(10)-C(15)-C(14)	120.6(3)	C(39)-C(34)-P(3)	116.9(3)
C(10)-C(15)-H(15)	119.7	C(36)-C(35)-C(34)	121.3(3)
C(14)-C(15)-H(15)	119.7	C(36)-C(35)-H(35)	119.3
C(17)-C(16)-C(21)	117.3(3)	C(34)-C(35)-H(35)	119.3
C(17)-C(16)-P(1)	119.9(3)	C(37)-C(36)-C(35)	119.9(3)
C(21)-C(16)-P(1)	122.8(3)	C(37)-C(36)-H(36)	120.1
C(18)-C(17)-C(16)	121.9(3)	C(35)-C(36)-H(36)	120.1
C(18)-C(17)-H(17)	119.1	C(36)-C(37)-C(38)	119.6(4)
C(16)-C(17)-H(17)	119.1	C(36)-C(37)-H(37)	120.2
C(17)-C(18)-C(19)	120.1(4)	C(38)-C(37)-H(37)	120.2
C(17)-C(18)-H(18)	119.9	C(39)-C(38)-C(37)	120.2(4)
C(19)-C(18)-H(18)	119.9	C(39)-C(38)-H(38)	119.9
C(20)-C(19)-C(18)	118.8(4)	C(37)-C(38)-H(38)	119.9
C(20)-C(19)-H(19)	120.6	C(38)-C(39)-C(34)	120.9(3)
C(18)-C(19)-H(19)	120.6	C(38)-C(39)-H(39)	119.5
C(21)-C(20)-C(19)	120.6(4)	C(34)-C(39)-H(39)	119.5
C(21)-C(20)-H(20)	119.7	C(45)-C(40)-C(41)	118.6(3)
C(19)-C(20)-H(20)	119.7	C(45)-C(40)-P(3)	121.6(3)
C(20)-C(21)-C(16)	121.3(4)	C(41)-C(40)-P(3)	119.7(3)
C(20)-C(21)-H(21)	119.4	C(42)-C(41)-C(40)	120.6(3)
C(16)-C(21)-H(21)	119.4	C(42)-C(41)-H(41)	119.7
C(23)-C(22)-C(27)	118.3(3)	C(40)-C(41)-H(41)	119.7
C(23)-C(22)-P(2)	124.0(3)	C(43)-C(42)-C(41)	120.2(4)
C(27)-C(22)-P(2)	117.8(3)	C(43)-C(42)-H(42)	119.9
C(24)-C(23)-C(22)	120.6(3)	C(41)-C(42)-H(42)	119.9
C(24)-C(23)-H(23)	119.7	C(44)-C(43)-C(42)	119.9(3)
C(22)-C(23)-H(23)	119.7	C(44)-C(43)-H(43)	120.0
C(23)-C(24)-C(25)	120.6(3)	C(42)-C(43)-H(43)	120.0
C(23)-C(24)-H(24)	119.7	C(43)-C(44)-C(45)	120.2(4)
C(25)-C(24)-H(24)	119.7	C(43)-C(44)-H(44)	119.9
C(26)-C(25)-C(24)	119.7(3)	C(45)-C(44)-H(44)	119.9
C(26)-C(25)-H(25)	120.1	C(40)-C(45)-C(44)	120.4(3)
C(24)-C(25)-H(25)	120.1	C(40)-C(45)-H(45)	119.8
C(25)-C(26)-C(27)	119.8(3)	C(44)-C(45)-H(45)	119.8
C(25)-C(26)-H(26)	120.1	C(51)-C(46)-C(47)	119.4(3)
C(27)-C(26)-H(26)	120.1	C(51)-C(46)-P(4)	124.7(3)
C(26)-C(27)-C(22)	120.9(3)	C(47)-C(46)-P(4)	115.9(3)
C(26)-C(27)-H(27)	119.6	C(46)-C(47)-C(48)	120.0(4)
C(22)-C(27)-H(27)	119.6	C(46)-C(47)-H(47)	120.0
C(29)-C(28)-C(33)	117.8(3)	C(48)-C(47)-H(47)	120.0

C(49)-C(48)-C(47)	119.8(4)	C(72)-C(71)-H(71A)	110.2
C(49)-C(48)-H(48)	120.1	C(75)-C(71)-H(71B)	110.2
C(47)-C(48)-H(48)	120.1	C(72)-C(71)-H(71B)	110.2
C(48)-C(49)-C(50)	120.4(4)	H(71A)-C(71)-H(71B)	108.5
C(48)-C(49)-H(49)	119.8	C(73)-C(72)-C(71)	110.1(5)
C(50)-C(49)-H(49)	119.8	C(73)-C(72)-H(72A)	109.6
C(49)-C(50)-C(51)	120.2(4)	C(71)-C(72)-H(72A)	109.6
C(49)-C(50)-H(50)	119.9	C(73)-C(72)-H(72B)	109.6
C(51)-C(50)-H(50)	119.9	C(71)-C(72)-H(72B)	109.6
C(46)-C(51)-C(50)	120.2(4)	H(72A)-C(72)-H(72B)	108.2
C(46)-C(51)-H(51)	119.9	C(72)-C(73)-C(74)	106.4(5)
C(50)-C(51)-H(51)	119.9	C(72)-C(73)-H(73A)	110.5
C(53)-C(52)-C(57)	118.3(3)	C(74)-C(73)-H(73A)	110.5
C(53)-C(52)-P(4)	123.5(3)	C(72)-C(73)-H(73B)	110.5
C(57)-C(52)-P(4)	118.0(3)	C(74)-C(73)-H(73B)	110.5
C(54)-C(53)-C(52)	120.5(4)	H(73A)-C(73)-H(73B)	108.6
C(54)-C(53)-H(53)	119.7	C(73)-C(74)-C(75)	109.2(5)
C(52)-C(53)-H(53)	119.7	C(73)-C(74)-H(74A)	109.8
C(53)-C(54)-C(55)	120.2(4)	C(75)-C(74)-H(74A)	109.8
C(53)-C(54)-H(54)	119.9	C(73)-C(74)-H(74B)	109.8
C(55)-C(54)-H(54)	119.9	C(75)-C(74)-H(74B)	109.8
C(56)-C(55)-C(54)	119.9(4)	H(74A)-C(74)-H(74B)	108.3
C(56)-C(55)-H(55)	120.0	C(71)-C(75)-C(74)	106.4(5)
C(54)-C(55)-H(55)	120.0	C(71)-C(75)-H(75A)	110.4
C(57)-C(56)-C(55)	119.5(4)	C(74)-C(75)-H(75A)	110.4
C(57)-C(56)-H(56)	120.3	C(71)-C(75)-H(75B)	110.4
C(55)-C(56)-H(56)	120.3	C(74)-C(75)-H(75B)	110.4
C(56)-C(57)-C(52)	121.6(4)	H(75A)-C(75)-H(75B)	108.6
C(56)-C(57)-H(57)	119.2	C(78)-C(77)-C(82)	120.0
C(52)-C(57)-H(57)	119.2	C(78)-C(77)-H(77)	120.0
C(59)-C(58)-C(63)	118.7(3)	C(82)-C(77)-H(77)	120.0
C(59)-C(58)-P(4)	124.0(3)	C(79)-C(78)-C(77)	120.0
C(63)-C(58)-P(4)	116.6(3)	C(79)-C(78)-H(78)	120.0
C(60)-C(59)-C(58)	120.3(4)	C(77)-C(78)-H(78)	120.0
C(60)-C(59)-H(59)	119.8	C(80)-C(79)-C(78)	120.0
C(58)-C(59)-H(59)	119.8	C(80)-C(79)-H(79)	120.0
C(61)-C(60)-C(59)	120.2(4)	C(78)-C(79)-H(79)	120.0
C(61)-C(60)-H(60)	119.9	C(79)-C(80)-C(81)	120.0
C(59)-C(60)-H(60)	119.9	C(79)-C(80)-H(80)	120.0
C(62)-C(61)-C(60)	120.0(4)	C(81)-C(80)-H(80)	120.0
C(62)-C(61)-H(61)	120.0	C(82)-C(81)-C(80)	120.0
C(60)-C(61)-H(61)	120.0	C(82)-C(81)-C(81)#1	97.8(12)
C(61)-C(62)-C(63)	120.2(4)	C(80)-C(81)-C(81)#1	116.8(12)
C(61)-C(62)-H(62)	119.9	C(82)-C(81)-H(81)	120.0
C(63)-C(62)-H(62)	119.9	C(80)-C(81)-H(81)	120.0
C(62)-C(63)-C(58)	120.6(4)	C(81)#1-C(81)-H(81)	54.1
C(62)-C(63)-H(63)	119.7	C(81)-C(82)-C(77)	120.0
C(58)-C(63)-H(63)	119.7	C(81)-C(82)-H(82)	120.0
C(75)-C(71)-C(72)	107.7(5)	C(77)-C(82)-H(82)	120.0
C(75)-C(71)-H(71A)	110.2		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $[PhBP_3]FePPh_3$ (CCDC 192834). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	230(3)	142(2)	145(2)	15(2)	-2(2)	-16(2)
P(1)	238(5)	138(4)	188(5)	18(4)	7(4)	5(4)
P(2)	218(5)	126(4)	172(5)	15(4)	-15(4)	-6(4)
P(3)	234(5)	150(4)	153(5)	7(4)	-11(4)	-29(4)
P(4)	310(6)	208(5)	162(5)	21(4)	13(4)	-26(5)
B(1)	260(20)	144(18)	150(20)	6(15)	-6(18)	12(18)
C(1)	230(20)	133(16)	189(18)	-3(14)	-29(16)	63(15)
C(2)	270(20)	163(17)	200(20)	-15(15)	-2(17)	14(16)
C(3)	410(30)	184(19)	230(20)	55(16)	33(18)	20(18)
C(4)	650(30)	290(20)	146(19)	46(16)	-20(20)	50(20)
C(5)	580(30)	270(20)	230(20)	-31(17)	-130(20)	-30(20)
C(6)	370(20)	168(18)	199(19)	35(15)	-44(17)	13(17)
C(7)	290(20)	122(16)	157(18)	4(14)	-18(16)	19(16)
C(8)	210(20)	147(17)	153(18)	-8(14)	15(15)	13(15)
C(9)	230(20)	161(17)	174(19)	26(14)	19(15)	25(15)
C(10)	260(20)	149(17)	200(20)	-35(15)	41(16)	13(15)
C(11)	260(20)	195(18)	230(20)	-3(16)	3(17)	32(16)
C(12)	390(20)	167(19)	320(20)	32(17)	10(18)	54(17)
C(13)	560(30)	146(19)	430(30)	-42(19)	90(20)	67(19)
C(14)	640(30)	280(20)	270(20)	-80(18)	70(20)	30(20)
C(15)	480(30)	188(19)	230(20)	27(16)	27(19)	0(19)
C(16)	210(20)	219(18)	200(20)	82(16)	-11(16)	16(16)
C(17)	230(20)	209(19)	310(20)	13(17)	-5(18)	16(16)
C(18)	310(20)	240(20)	410(30)	51(18)	10(20)	-27(18)
C(19)	250(20)	320(20)	410(30)	130(20)	12(19)	-19(19)
C(20)	290(30)	340(20)	550(30)	10(20)	100(20)	80(20)
C(21)	280(20)	240(20)	510(30)	-62(19)	80(20)	-41(18)
C(22)	200(20)	97(16)	230(20)	7(14)	-18(15)	21(14)
C(23)	220(20)	173(17)	230(20)	-28(15)	-15(16)	30(16)
C(24)	240(20)	186(18)	250(20)	-76(16)	-54(17)	17(16)
C(25)	240(20)	177(19)	390(20)	-40(17)	-68(18)	-18(16)
C(26)	260(20)	198(19)	280(20)	20(17)	34(17)	-42(16)
C(27)	270(20)	201(18)	220(20)	-10(16)	-44(17)	-21(16)
C(28)	270(20)	142(17)	152(18)	-27(14)	-16(16)	29(15)
C(29)	250(20)	174(18)	300(20)	54(16)	3(17)	21(16)
C(30)	230(20)	270(20)	430(20)	-38(19)	-17(19)	21(18)
C(31)	290(20)	200(20)	390(20)	-53(18)	-87(19)	93(17)
C(32)	330(20)	134(17)	290(20)	6(16)	-68(18)	33(17)
C(33)	220(20)	182(18)	240(20)	-14(15)	-18(16)	-30(15)
C(34)	200(20)	162(18)	200(20)	-12(15)	-11(16)	-38(15)
C(35)	310(20)	190(18)	190(20)	25(15)	7(17)	-30(17)
C(36)	300(20)	250(20)	330(20)	-9(18)	101(19)	-44(18)
C(37)	200(20)	360(20)	500(30)	-10(20)	10(20)	16(18)
C(38)	290(20)	440(30)	410(30)	200(20)	-40(20)	-30(20)
C(39)	180(20)	350(20)	270(20)	82(18)	32(16)	-9(18)
C(40)	260(20)	163(17)	157(18)	-7(15)	11(16)	-52(15)
C(41)	360(20)	206(18)	180(20)	-1(16)	-31(17)	-31(17)
C(42)	440(30)	185(19)	270(20)	-11(16)	16(19)	-23(18)

C(43)	500(30)	210(20)	310(20)	-60(17)	60(20)	-120(20)
C(44)	390(30)	370(20)	340(30)	-70(20)	-100(20)	-120(20)
C(45)	330(20)	210(20)	270(20)	-23(17)	-23(18)	-49(17)
C(46)	450(30)	231(19)	172(19)	28(15)	-15(19)	-1(19)
C(47)	990(40)	390(30)	220(20)	-69(19)	80(20)	-270(30)
C(48)	1590(60)	390(30)	300(30)	-90(20)	140(30)	-420(30)
C(49)	1380(50)	330(20)	230(20)	-64(19)	60(30)	-50(30)
C(50)	890(40)	330(20)	230(20)	16(19)	120(20)	80(20)
C(51)	570(30)	220(20)	240(20)	12(17)	70(20)	50(20)
C(52)	250(20)	310(20)	138(19)	46(16)	33(16)	-31(17)
C(53)	280(20)	450(20)	190(20)	-25(18)	68(18)	-50(20)
C(54)	270(20)	760(30)	240(20)	-100(20)	28(19)	20(20)
C(55)	270(30)	870(40)	310(30)	-30(20)	50(20)	200(30)
C(56)	370(30)	520(30)	290(20)	-20(20)	80(20)	150(20)
C(57)	330(20)	370(20)	190(20)	46(17)	13(18)	15(19)
C(58)	290(20)	290(20)	141(19)	-15(15)	40(17)	-32(18)
C(59)	390(20)	270(20)	160(20)	22(15)	30(18)	-38(19)
C(60)	540(30)	350(20)	270(20)	-17(19)	90(20)	-130(20)
C(61)	440(30)	610(30)	320(30)	-80(20)	90(20)	-250(30)
C(62)	290(30)	690(30)	350(30)	0(20)	-20(20)	-30(20)
C(63)	350(30)	390(20)	240(20)	57(18)	30(19)	20(20)
C(71)	1910(150)	4600(300)	8100(400)	5600(300)	0(200)	-720(170)
C(72)	5500(180)	6800(200)	5300(300)	5580(180)	-4580(170)	-5670
C(73)	1190(110)	3110(160)	5800(300)	2690(180)	-810(140)	-660(110)
C(74)	1160(110)	7000(400)	6600(400)	5800(300)	-1030(170)	-1130(170)
C(75)	3180(190)	1760(100)	2050(100)	1010(90)	-930(130)	-2180(120)
C(77)	1140(120)	1700(150)	740(100)	-280(100)	200(90)	-360(110)
C(78)	540(90)	3300(200)	870(110)	-840(140)	40(80)	920(120)
C(79)	660(90)	1900(150)	780(100)	-150(90)	220(80)	750(100)
C(80)	1660(150)	580(80)	1190(120)	-440(80)	-780(110)	520(90)
C(81)	9400(700)	330(100)	1400(200)	420(100)	-2400(300)	-1000(200)
C(82)	4700(400)	2200(200)	1550(170)	930(150)	-2000(200)	-2600(200)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FePPh_3$ (CCDC 192834).

	x	y	z	U_{iso}
H(2)	4303	7502	3050	26
H(3)	4354	7320	3734	33
H(4)	4976	8121	4133	44
H(5)	5571	9106	3829	43
H(6)	5512	9293	3147	30
H(7A)	5892	8062	2533	23
H(7B)	5929	8957	2498	23
H(8A)	4756	9745	2691	20
H(8B)	4116	9397	2486	20
H(9A)	4020	7867	2451	22
H(9B)	4667	7437	2303	22
H(11)	6063	6963	2296	27
H(12)	6166	5715	2091	35
H(13)	6160	5417	1417	46
H(14)	6012	6368	937	48
H(15)	5860	7616	1144	36
H(17)	6703	9668	2123	30
H(18)	7802	10010	2093	38
H(19)	8572	9214	1784	40
H(20)	8209	8075	1505	47
H(21)	7103	7749	1525	41
H(23)	5511	10559	2706	25
H(24)	6474	11248	2785	27
H(25)	7096	11609	2230	32
H(26)	6733	11302	1590	30
H(27)	5785	10577	1507	28
H(29)	3377	10014	2119	29
H(30)	2573	10930	2035	37
H(31)	2860	12145	1826	35
H(32)	3964	12442	1715	30
H(33)	4776	11526	1799	26
H(35)	3019	8172	2292	28
H(36)	1983	8722	2229	35
H(37)	1743	9468	1676	42
H(38)	2551	9659	1182	46
H(39)	3579	9108	1244	32
H(41)	4817	6654	1741	30
H(42)	4592	5519	1415	36
H(43)	3625	5383	1043	41
H(44)	2894	6388	986	44
H(45)	3126	7541	1299	33
H(47)	4563	7823	885	64
H(48)	4544	6782	452	91
H(49)	5050	6859	-165	77
H(50)	5591	7954	-356	58
H(51)	5619	8990	73	41
H(53)	4050	9171	238	37
H(54)	3117	9873	70	51

H(55)	2870	10982	416	58
H(56)	3545	11372	947	47
H(57)	4466	10674	1114	35
H(59)	5362	10816	550	33
H(60)	6322	11535	535	46
H(61)	7325	11012	738	55
H(62)	7367	9759	955	53
H(63)	6413	9037	976	39
H(71A)	6980	3377	67	585
H(71B)	6625	2705	306	585
H(72A)	6717	1962	-210	705
H(72B)	7016	2654	-460	705
H(73A)	7981	2123	-463	405
H(73B)	7673	1410	-232	405
H(74A)	8497	2459	81	591
H(74B)	8190	1748	312	591
H(75A)	7521	2502	654	279
H(75B)	7856	3218	439	279
H(77)	8284	10044	-367	143
H(78)	7952	9420	216	189
H(79)	8688	9292	751	134
H(80)	9756	9787	703	137
H(81)	10088	10411	120	449
H(82)	9352	10539	-414	336

Table 11. Crystal data and structure refinement for $[PhBP_3]FeNTol \cdot C_6H_6$.

Identification code	sdb17	
Empirical formula	$C_{55}H_{51}BFeNP_3$	
Formula weight	885.54	
Crystal Habit	irregular	
Crystal Color	deep green	
Crystal size	0.074 x 0.25 x 0.27 mm^3	
Type of diffractometer	Bruker P4	
Wavelength	0.71073 Å	
Data collection temperature	98(2) K	
Unit cell dimensions	a = 10.9216(8) Å	α= 85.0390(10)°.
	b = 16.9009(13) Å	β= 85.4520(10)°.
	c = 25.2795(19) Å	γ = 77.0040(10)°.
Volume	4521.0(6) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.301 Mg/m^3	
F(000)	1856	
Theta range for data collection	1.24 to 28.66°.	
Completeness to theta = 28.66°	92.2 %	
Index ranges	-14<=h<=14, -22<=k<=22, -33<=l<=33	
Reflections collected	96972	
Independent reflections	21438 [R(int) = 0.0880]	
Absorption coefficient	0.479 mm^{-1}	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21438 / 0 / 1153	
Goodness-of-fit on F^2	1.218	
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.0806	
R indices (all data)	R1 = 0.1006, wR2 = 0.0915	
Largest diff. peak and hole	0.676 and -0.552 $e.Å^{-3}$	

Special Refinement Details

The crystal contains benzene located in one site in two conformations (½ per asymmetric unit). The benzene molecule was modeled in the two positions while refining the relative population distribution.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FeNTol{\cdot}C_6H_6$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	1350(1)	8121(1)	4108(1)	18(1)
P(1)	-251(1)	9009(1)	3708(1)	17(1)
P(2)	588(1)	7060(1)	3940(1)	18(1)
P(3)	2390(1)	7998(1)	3317(1)	18(1)
N(1)	2144(2)	8078(1)	4646(1)	19(1)
B(1)	43(3)	7862(2)	2887(1)	18(1)
C(1)	-589(2)	7765(1)	2336(1)	20(1)
C(2)	-153(2)	8055(2)	1834(1)	24(1)
C(3)	-728(3)	8020(2)	1372(1)	29(1)
C(4)	-1787(3)	7696(2)	1388(1)	31(1)
C(5)	-2248(3)	7401(2)	1873(1)	30(1)
C(6)	-1656(2)	7437(2)	2332(1)	24(1)
C(7)	-508(2)	8818(1)	3037(1)	19(1)
C(8)	-365(2)	7217(1)	3370(1)	20(1)
C(9)	1605(2)	7686(1)	2792(1)	19(1)
C(10)	-1728(2)	9011(1)	4108(1)	19(1)
C(11)	-2772(2)	8813(2)	3918(1)	28(1)
C(12)	-3868(2)	8857(2)	4244(1)	35(1)
C(13)	-3943(3)	9097(2)	4752(1)	36(1)
C(14)	-2909(3)	9292(2)	4944(1)	33(1)
C(15)	-1802(2)	9239(2)	4627(1)	26(1)
C(16)	-191(2)	10085(1)	3702(1)	17(1)
C(17)	472(2)	10352(2)	4073(1)	22(1)
C(18)	483(2)	11170(2)	4081(1)	25(1)
C(19)	-163(2)	11728(2)	3713(1)	24(1)
C(20)	-821(2)	11473(2)	3344(1)	24(1)
C(21)	-842(2)	10658(2)	3334(1)	21(1)
C(22)	-335(2)	6688(1)	4506(1)	18(1)
C(23)	-933(2)	6061(2)	4454(1)	28(1)
C(24)	-1578(2)	5749(2)	4887(1)	30(1)
C(25)	-1650(2)	6067(2)	5373(1)	27(1)
C(26)	-1079(2)	6702(2)	5427(1)	28(1)
C(27)	-415(2)	7010(2)	4995(1)	26(1)
C(28)	1847(2)	6158(1)	3834(1)	20(1)
C(29)	1991(2)	5717(2)	3388(1)	26(1)
C(30)	3023(3)	5082(2)	3308(1)	35(1)
C(31)	3925(3)	4881(2)	3674(1)	37(1)
C(32)	3787(3)	5297(2)	4128(1)	37(1)
C(33)	2750(2)	5933(2)	4210(1)	27(1)
C(34)	3978(2)	7356(1)	3314(1)	20(1)
C(35)	4685(2)	7342(2)	3749(1)	30(1)
C(36)	5897(3)	6872(2)	3773(1)	37(1)
C(37)	6405(3)	6390(2)	3361(1)	38(1)
C(38)	5724(3)	6401(2)	2925(1)	41(1)
C(39)	4516(3)	6885(2)	2903(1)	34(1)
C(40)	2693(2)	9011(1)	3115(1)	19(1)
C(41)	2434(2)	9426(2)	2624(1)	30(1)
C(42)	2623(3)	10212(2)	2523(1)	35(1)
C(43)	3074(2)	10584(2)	2905(1)	31(1)
C(44)	3366(2)	10170(2)	3389(1)	28(1)
C(45)	3157(2)	9393(2)	3493(1)	25(1)

C(46)	2986(2)	7978(2)	5040(1)	20(1)
C(47)	4011(2)	7306(2)	5076(1)	26(1)
C(48)	4897(2)	7264(2)	5442(1)	28(1)
C(49)	4807(2)	7875(2)	5785(1)	27(1)
C(50)	3762(2)	8517(2)	5770(1)	28(1)
C(51)	2865(2)	8568(2)	5406(1)	25(1)
C(52)	5854(3)	7849(2)	6145(1)	36(1)
Fe(2)	5521(1)	3120(1)	1202(1)	16(1)
N(2)	4774(2)	2690(1)	799(1)	19(1)
P(4)	7574(1)	3003(1)	1284(1)	16(1)
P(5)	5426(1)	2477(1)	1998(1)	16(1)
P(6)	5077(1)	4327(1)	1571(1)	16(1)
B(2)	6887(2)	3581(2)	2362(1)	16(1)
C(53)	7522(2)	3819(1)	2871(1)	18(1)
C(54)	8328(2)	4366(2)	2805(1)	25(1)
C(55)	8895(2)	4589(2)	3226(1)	28(1)
C(56)	8662(3)	4278(2)	3736(1)	31(1)
C(57)	7867(3)	3750(2)	3819(1)	34(1)
C(58)	7316(2)	3525(2)	3396(1)	25(1)
C(59)	7993(2)	3429(1)	1863(1)	18(1)
C(60)	6328(2)	2750(1)	2504(1)	17(1)
C(61)	5681(2)	4339(1)	2218(1)	17(1)
C(62)	8343(2)	3447(1)	698(1)	18(1)
C(63)	7747(2)	3638(2)	225(1)	27(1)
C(64)	8353(3)	3952(2)	-224(1)	31(1)
C(65)	9541(2)	4077(2)	-198(1)	29(1)
C(66)	10142(2)	3897(2)	269(1)	28(1)
C(67)	9551(2)	3577(1)	714(1)	22(1)
C(68)	8437(2)	1943(1)	1288(1)	18(1)
C(69)	8540(2)	1542(2)	822(1)	23(1)
C(70)	9114(2)	726(2)	813(1)	30(1)
C(71)	9590(2)	297(2)	1269(1)	35(1)
C(72)	9510(2)	679(2)	1731(1)	33(1)
C(73)	8938(2)	1504(2)	1740(1)	23(1)
C(74)	5854(2)	1362(1)	2019(1)	18(1)
C(75)	6017(2)	945(2)	1563(1)	23(1)
C(76)	6334(2)	99(2)	1595(1)	30(1)
C(77)	6487(2)	-333(2)	2083(1)	30(1)
C(78)	6315(2)	81(2)	2539(1)	28(1)
C(79)	6009(2)	917(2)	2510(1)	24(1)
C(80)	3774(2)	2644(1)	2248(1)	17(1)
C(81)	2979(2)	2279(2)	1995(1)	23(1)
C(82)	1705(2)	2419(2)	2141(1)	25(1)
C(83)	1203(2)	2918(2)	2549(1)	27(1)
C(84)	1982(2)	3280(2)	2803(1)	26(1)
C(85)	3261(2)	3144(2)	2651(1)	21(1)
C(86)	3406(2)	4827(1)	1625(1)	17(1)
C(87)	2478(2)	4446(2)	1497(1)	23(1)
C(88)	1215(2)	4832(2)	1555(1)	27(1)
C(89)	868(2)	5595(2)	1741(1)	28(1)
C(90)	1776(3)	5980(2)	1866(1)	33(1)
C(91)	3034(2)	5602(2)	1813(1)	28(1)
C(92)	5745(2)	5078(1)	1146(1)	18(1)
C(93)	5255(2)	5344(2)	655(1)	26(1)
C(94)	5727(3)	5915(2)	322(1)	31(1)
C(95)	6713(2)	6217(2)	473(1)	29(1)

C(96)	7219(2)	5950(2)	954(1)	27(1)
C(97)	6729(2)	5389(1)	1290(1)	22(1)
C(98)	2227(3)	656(2)	-176(1)	34(1)
C(99)	4149(2)	2210(1)	560(1)	19(1)
C(100)	4803(2)	1636(2)	212(1)	24(1)
C(101)	4182(3)	1146(2)	-24(1)	26(1)
C(102)	2888(3)	1203(2)	77(1)	25(1)
C(103)	2238(2)	1781(2)	415(1)	25(1)
C(104)	2851(2)	2281(2)	651(1)	21(1)
C(108)	7810(20)	1275(15)	9209(9)	40(5)
C(109)	6980(30)	792(19)	8921(12)	70(10)
C(111)	5820(20)	2310(20)	8729(8)	52(9)
C(112)	6530(30)	2560(13)	8996(12)	66(8)
C(113)	7499(14)	2089(11)	9247(6)	40(4)
C(110)	6051(13)	1347(8)	8665(5)	54(5)
C(119)	7521(13)	1405(8)	9210(5)	60(6)
C(114)	7209(14)	844(8)	9008(7)	30(3)
C(116)	5623(9)	1721(6)	8552(4)	52(3)
C(117)	5970(20)	2307(15)	8720(9)	100(12)
C(118)	6924(13)	2217(9)	9055(7)	68(7)
C(115)	6220(10)	909(6)	8679(5)	50(3)

Table 13. Bond lengths [Å] and angles [°] for $[PhBP_3]FeNTol \cdot C_6H_6$.

Fe(1)-N(1)	1.659(2)	C(20)-C(21)	1.385(3)
Fe(1)-P(3)	2.2229(7)	C(20)-H(20)	0.9500
Fe(1)-P(2)	2.2234(7)	C(21)-H(21)	0.9500
Fe(1)-P(1)	2.2733(7)	C(22)-C(27)	1.381(3)
P(1)-C(7)	1.810(2)	C(22)-C(23)	1.384(3)
P(1)-C(16)	1.832(2)	C(23)-C(24)	1.385(3)
P(1)-C(10)	1.834(2)	C(23)-H(23)	0.9500
P(2)-C(8)	1.811(2)	C(24)-C(25)	1.371(3)
P(2)-C(28)	1.832(2)	C(24)-H(24)	0.9500
P(2)-C(22)	1.834(2)	C(25)-C(26)	1.379(3)
P(3)-C(9)	1.810(2)	C(25)-H(25)	0.9500
P(3)-C(34)	1.828(3)	C(26)-C(27)	1.392(3)
P(3)-C(40)	1.837(2)	C(26)-H(26)	0.9500
N(1)-C(46)	1.382(3)	C(27)-H(27)	0.9500
B(1)-C(1)	1.638(4)	C(28)-C(29)	1.385(3)
B(1)-C(7)	1.658(4)	C(28)-C(33)	1.394(3)
B(1)-C(9)	1.666(4)	C(29)-C(30)	1.386(3)
B(1)-C(8)	1.667(3)	C(29)-H(29)	0.9500
C(1)-C(6)	1.400(3)	C(30)-C(31)	1.373(4)
C(1)-C(2)	1.405(3)	C(30)-H(30)	0.9500
C(2)-C(3)	1.381(3)	C(31)-C(32)	1.378(4)
C(2)-H(2)	0.9500	C(31)-H(31)	0.9500
C(3)-C(4)	1.383(4)	C(32)-C(33)	1.391(4)
C(3)-H(3)	0.9500	C(32)-H(32)	0.9500
C(4)-C(5)	1.384(4)	C(33)-H(33)	0.9500
C(4)-H(4)	0.9500	C(34)-C(39)	1.375(3)
C(5)-C(6)	1.387(3)	C(34)-C(35)	1.388(3)
C(5)-H(5)	0.9500	C(35)-C(36)	1.385(3)
C(6)-H(6)	0.9500	C(35)-H(35)	0.9500
C(7)-H(7A)	0.9900	C(36)-C(37)	1.382(4)
C(7)-H(7B)	0.9900	C(36)-H(36)	0.9500
C(8)-H(8A)	0.9900	C(37)-C(38)	1.373(4)
C(8)-H(8B)	0.9900	C(37)-H(37)	0.9500
C(9)-H(9A)	0.9900	C(38)-C(39)	1.390(4)
C(9)-H(9B)	0.9900	C(38)-H(38)	0.9500
C(10)-C(11)	1.388(3)	C(39)-H(39)	0.9500
C(10)-C(15)	1.390(3)	C(40)-C(45)	1.385(3)
C(11)-C(12)	1.388(4)	C(40)-C(41)	1.388(3)
C(11)-H(11)	0.9500	C(41)-C(42)	1.389(3)
C(12)-C(13)	1.371(4)	C(41)-H(41)	0.9500
C(12)-H(12)	0.9500	C(42)-C(43)	1.376(4)
C(13)-C(14)	1.379(4)	C(42)-H(42)	0.9500
C(13)-H(13)	0.9500	C(43)-C(44)	1.378(3)
C(14)-C(15)	1.386(3)	C(43)-H(43)	0.9500
C(14)-H(14)	0.9500	C(44)-C(45)	1.382(3)
C(15)-H(15)	0.9500	C(44)-H(44)	0.9500
C(16)-C(17)	1.391(3)	C(45)-H(45)	0.9500
C(16)-C(21)	1.396(3)	C(46)-C(51)	1.396(3)
C(17)-C(18)	1.388(3)	C(46)-C(47)	1.406(3)
C(17)-H(17)	0.9500	C(47)-C(48)	1.376(3)
C(18)-C(19)	1.379(3)	C(47)-H(47)	0.9500
C(18)-H(18)	0.9500	C(48)-C(49)	1.387(4)
C(19)-C(20)	1.375(3)	C(48)-H(48)	0.9500
C(19)-H(19)	0.9500	C(49)-C(50)	1.387(3)

C(49)-C(52)	1.506(3)	C(69)-H(69)	0.9500
C(50)-C(51)	1.381(3)	C(70)-C(71)	1.380(4)
C(50)-H(50)	0.9500	C(70)-H(70)	0.9500
C(51)-H(51)	0.9500	C(71)-C(72)	1.370(4)
C(52)-H(52A)	0.9800	C(71)-H(71)	0.9500
C(52)-H(52B)	0.9800	C(72)-C(73)	1.395(3)
C(52)-H(52C)	0.9800	C(72)-H(72)	0.9500
Fe(2)-N(2)	1.661(2)	C(73)-H(73)	0.9500
Fe(2)-P(5)	2.2097(7)	C(74)-C(75)	1.383(3)
Fe(2)-P(4)	2.2312(7)	C(74)-C(79)	1.395(3)
Fe(2)-P(6)	2.2543(7)	C(75)-C(76)	1.390(3)
N(2)-C(99)	1.374(3)	C(75)-H(75)	0.9500
P(4)-C(59)	1.820(2)	C(76)-C(77)	1.380(3)
P(4)-C(68)	1.827(2)	C(76)-H(76)	0.9500
P(4)-C(62)	1.831(2)	C(77)-C(78)	1.378(4)
P(5)-C(60)	1.824(2)	C(77)-H(77)	0.9500
P(5)-C(80)	1.833(2)	C(78)-C(79)	1.375(3)
P(5)-C(74)	1.833(2)	C(78)-H(78)	0.9500
P(6)-C(61)	1.815(2)	C(79)-H(79)	0.9500
P(6)-C(86)	1.830(2)	C(80)-C(85)	1.383(3)
P(6)-C(92)	1.831(2)	C(80)-C(81)	1.393(3)
B(2)-C(53)	1.629(4)	C(81)-C(82)	1.383(3)
B(2)-C(60)	1.655(3)	C(81)-H(81)	0.9500
B(2)-C(61)	1.656(3)	C(82)-C(83)	1.388(4)
B(2)-C(59)	1.669(3)	C(82)-H(82)	0.9500
C(53)-C(58)	1.396(3)	C(83)-C(84)	1.379(3)
C(53)-C(54)	1.406(3)	C(83)-H(83)	0.9500
C(54)-C(55)	1.392(3)	C(84)-C(85)	1.391(3)
C(54)-H(54)	0.9500	C(84)-H(84)	0.9500
C(55)-C(56)	1.378(4)	C(85)-H(85)	0.9500
C(55)-H(55)	0.9500	C(86)-C(87)	1.389(3)
C(56)-C(57)	1.371(4)	C(86)-C(91)	1.394(3)
C(56)-H(56)	0.9500	C(87)-C(88)	1.389(3)
C(57)-C(58)	1.390(3)	C(87)-H(87)	0.9500
C(57)-H(57)	0.9500	C(88)-C(89)	1.372(3)
C(58)-H(58)	0.9500	C(88)-H(88)	0.9500
C(59)-H(59A)	0.9900	C(89)-C(90)	1.372(4)
C(59)-H(59B)	0.9900	C(89)-H(89)	0.9500
C(60)-H(60A)	0.9900	C(90)-C(91)	1.380(3)
C(60)-H(60B)	0.9900	C(90)-H(90)	0.9500
C(61)-H(61A)	0.9900	C(91)-H(91)	0.9500
C(61)-H(61B)	0.9900	C(92)-C(97)	1.384(3)
C(62)-C(63)	1.384(3)	C(92)-C(93)	1.390(3)
C(62)-C(67)	1.390(3)	C(93)-C(94)	1.384(3)
C(63)-C(64)	1.395(3)	C(93)-H(93)	0.9500
C(63)-H(63)	0.9500	C(94)-C(95)	1.382(4)
C(64)-C(65)	1.369(3)	C(94)-H(94)	0.9500
C(64)-H(64)	0.9500	C(95)-C(96)	1.374(3)
C(65)-C(66)	1.374(3)	C(95)-H(95)	0.9500
C(65)-H(65)	0.9500	C(96)-C(97)	1.387(3)
C(66)-C(67)	1.382(3)	C(96)-H(96)	0.9500
C(66)-H(66)	0.9500	C(97)-H(97)	0.9500
C(67)-H(67)	0.9500	C(98)-C(102)	1.505(3)
C(68)-C(73)	1.387(3)	C(98)-H(98A)	0.9800
C(68)-C(69)	1.394(3)	C(98)-H(98B)	0.9800
C(69)-C(70)	1.382(3)	C(98)-H(98C)	0.9800

C(99)-C(104)	1.398(3)	C(34)-P(3)-C(40)	102.34(11)
C(99)-C(100)	1.400(3)	C(9)-P(3)-Fe(1)	116.99(8)
C(100)-C(101)	1.379(3)	C(34)-P(3)-Fe(1)	115.70(8)
C(100)-H(100)	0.9500	C(40)-P(3)-Fe(1)	105.30(8)
C(101)-C(102)	1.399(3)	C(46)-N(1)-Fe(1)	169.99(18)
C(101)-H(101)	0.9500	C(1)-B(1)-C(7)	106.27(19)
C(102)-C(103)	1.386(4)	C(1)-B(1)-C(9)	110.3(2)
C(103)-C(104)	1.387(3)	C(7)-B(1)-C(9)	109.38(19)
C(103)-H(103)	0.9500	C(1)-B(1)-C(8)	109.99(19)
C(104)-H(104)	0.9500	C(7)-B(1)-C(8)	110.8(2)
C(108)-C(113)	1.35(3)	C(9)-B(1)-C(8)	110.05(19)
C(108)-C(109)	1.60(3)	C(6)-C(1)-C(2)	114.9(2)
C(108)-H(108)	0.9500	C(6)-C(1)-B(1)	122.5(2)
C(108)-H(119)	0.7763	C(2)-C(1)-B(1)	122.5(2)
C(109)-C(110)	1.38(3)	C(3)-C(2)-C(1)	122.8(2)
C(109)-H(109)	0.9500	C(3)-C(2)-H(2)	118.6
C(111)-C(112)	1.23(5)	C(1)-C(2)-H(2)	118.6
C(111)-C(110)	1.61(4)	C(2)-C(3)-C(4)	120.4(3)
C(111)-H(111)	0.9500	C(2)-C(3)-H(3)	119.8
C(112)-C(113)	1.34(4)	C(4)-C(3)-H(3)	119.8
C(112)-H(112)	0.9500	C(3)-C(4)-C(5)	118.8(2)
C(113)-H(113)	0.9500	C(3)-C(4)-H(4)	120.6
C(113)-H(119)	1.4522	C(5)-C(4)-H(4)	120.6
C(110)-H(110)	0.9500	C(4)-C(5)-C(6)	120.0(3)
C(119)-C(114)	1.24(2)	C(4)-C(5)-H(5)	120.0
C(119)-C(118)	1.416(19)	C(6)-C(5)-H(5)	120.0
C(119)-H(119)	0.9500	C(5)-C(6)-C(1)	123.0(2)
C(114)-C(115)	1.39(2)	C(5)-C(6)-H(6)	118.5
C(114)-H(114)	0.9500	C(1)-C(6)-H(6)	118.5
C(116)-C(117)	1.25(3)	B(1)-C(7)-P(1)	114.26(16)
C(116)-C(115)	1.403(11)	B(1)-C(7)-H(7A)	108.7
C(116)-H(116)	0.9500	P(1)-C(7)-H(7A)	108.7
C(117)-C(118)	1.37(3)	B(1)-C(7)-H(7B)	108.7
C(117)-H(117)	0.9500	P(1)-C(7)-H(7B)	108.7
C(118)-H(118)	0.9500	H(7A)-C(7)-H(7B)	107.6
C(115)-H(115)	0.9500	B(1)-C(8)-P(2)	114.32(16)
N(1)-Fe(1)-P(3)	119.36(7)	B(1)-C(8)-H(8A)	108.7
N(1)-Fe(1)-P(2)	119.83(7)	P(2)-C(8)-H(8A)	108.7
P(3)-Fe(1)-P(2)	86.89(3)	B(1)-C(8)-H(8B)	108.7
N(1)-Fe(1)-P(1)	136.91(7)	P(2)-C(8)-H(8B)	108.7
P(3)-Fe(1)-P(1)	88.46(3)	H(8A)-C(8)-H(8B)	107.6
P(2)-Fe(1)-P(1)	91.77(3)	B(1)-C(9)-P(3)	114.53(16)
C(7)-P(1)-C(16)	107.12(11)	B(1)-C(9)-H(9A)	108.6
C(7)-P(1)-C(10)	107.13(11)	P(3)-C(9)-H(9A)	108.6
C(16)-P(1)-C(10)	100.41(11)	B(1)-C(9)-H(9B)	108.6
C(7)-P(1)-Fe(1)	116.22(8)	P(3)-C(9)-H(9B)	108.6
C(16)-P(1)-Fe(1)	115.22(8)	H(9A)-C(9)-H(9B)	107.6
C(10)-P(1)-Fe(1)	109.33(8)	C(11)-C(10)-C(15)	118.7(2)
C(8)-P(2)-C(28)	106.80(12)	C(11)-C(10)-P(1)	123.8(2)
C(8)-P(2)-C(22)	107.31(11)	C(15)-C(10)-P(1)	117.48(19)
C(28)-P(2)-C(22)	101.26(11)	C(10)-C(11)-C(12)	119.9(3)
C(8)-P(2)-Fe(1)	115.26(8)	C(10)-C(11)-H(11)	120.0
C(28)-P(2)-Fe(1)	111.63(8)	C(12)-C(11)-H(11)	120.0
C(22)-P(2)-Fe(1)	113.45(8)	C(13)-C(12)-C(11)	121.1(3)
C(9)-P(3)-C(34)	106.83(11)	C(13)-C(12)-H(12)	119.4
C(9)-P(3)-C(40)	108.49(11)	C(11)-C(12)-H(12)	119.4

C(12)-C(13)-C(14)	119.3(3)	C(32)-C(31)-H(31)	120.0
C(12)-C(13)-H(13)	120.3	C(31)-C(32)-C(33)	120.1(3)
C(14)-C(13)-H(13)	120.3	C(31)-C(32)-H(32)	119.9
C(13)-C(14)-C(15)	120.2(3)	C(33)-C(32)-H(32)	119.9
C(13)-C(14)-H(14)	119.9	C(32)-C(33)-C(28)	120.5(3)
C(15)-C(14)-H(14)	119.9	C(32)-C(33)-H(33)	119.8
C(14)-C(15)-C(10)	120.7(2)	C(28)-C(33)-H(33)	119.8
C(14)-C(15)-H(15)	119.7	C(39)-C(34)-C(35)	118.0(2)
C(10)-C(15)-H(15)	119.7	C(39)-C(34)-P(3)	123.6(2)
C(17)-C(16)-C(21)	118.6(2)	C(35)-C(34)-P(3)	118.42(19)
C(17)-C(16)-P(1)	120.82(18)	C(36)-C(35)-C(34)	121.6(3)
C(21)-C(16)-P(1)	120.59(18)	C(36)-C(35)-H(35)	119.2
C(18)-C(17)-C(16)	120.9(2)	C(34)-C(35)-H(35)	119.2
C(18)-C(17)-H(17)	119.6	C(37)-C(36)-C(35)	119.2(3)
C(16)-C(17)-H(17)	119.6	C(37)-C(36)-H(36)	120.4
C(19)-C(18)-C(17)	119.7(2)	C(35)-C(36)-H(36)	120.4
C(19)-C(18)-H(18)	120.1	C(38)-C(37)-C(36)	120.0(3)
C(17)-C(18)-H(18)	120.1	C(38)-C(37)-H(37)	120.0
C(20)-C(19)-C(18)	120.0(2)	C(36)-C(37)-H(37)	120.0
C(20)-C(19)-H(19)	120.0	C(37)-C(38)-C(39)	120.0(3)
C(18)-C(19)-H(19)	120.0	C(37)-C(38)-H(38)	120.0
C(19)-C(20)-C(21)	120.6(2)	C(39)-C(38)-H(38)	120.0
C(19)-C(20)-H(20)	119.7	C(34)-C(39)-C(38)	121.2(3)
C(21)-C(20)-H(20)	119.7	C(34)-C(39)-H(39)	119.4
C(20)-C(21)-C(16)	120.1(2)	C(38)-C(39)-H(39)	119.4
C(20)-C(21)-H(21)	119.9	C(45)-C(40)-C(41)	118.6(2)
C(16)-C(21)-H(21)	119.9	C(45)-C(40)-P(3)	116.83(18)
C(27)-C(22)-C(23)	118.9(2)	C(41)-C(40)-P(3)	124.5(2)
C(27)-C(22)-P(2)	120.74(19)	C(40)-C(41)-C(42)	120.1(3)
C(23)-C(22)-P(2)	120.33(19)	C(40)-C(41)-H(41)	120.0
C(22)-C(23)-C(24)	120.7(2)	C(42)-C(41)-H(41)	120.0
C(22)-C(23)-H(23)	119.7	C(43)-C(42)-C(41)	120.5(3)
C(24)-C(23)-H(23)	119.7	C(43)-C(42)-H(42)	119.8
C(25)-C(24)-C(23)	120.3(2)	C(41)-C(42)-H(42)	119.8
C(25)-C(24)-H(24)	119.9	C(42)-C(43)-C(44)	119.9(3)
C(23)-C(24)-H(24)	119.9	C(42)-C(43)-H(43)	120.0
C(24)-C(25)-C(26)	119.6(2)	C(44)-C(43)-H(43)	120.0
C(24)-C(25)-H(25)	120.2	C(43)-C(44)-C(45)	119.6(3)
C(26)-C(25)-H(25)	120.2	C(43)-C(44)-H(44)	120.2
C(25)-C(26)-C(27)	120.2(2)	C(45)-C(44)-H(44)	120.2
C(25)-C(26)-H(26)	119.9	C(44)-C(45)-C(40)	121.3(2)
C(27)-C(26)-H(26)	119.9	C(44)-C(45)-H(45)	119.3
C(22)-C(27)-C(26)	120.3(2)	C(40)-C(45)-H(45)	119.3
C(22)-C(27)-H(27)	119.9	N(1)-C(46)-C(51)	120.3(2)
C(26)-C(27)-H(27)	119.9	N(1)-C(46)-C(47)	122.0(2)
C(29)-C(28)-C(33)	118.2(2)	C(51)-C(46)-C(47)	117.7(2)
C(29)-C(28)-P(2)	123.8(2)	C(48)-C(47)-C(46)	120.5(2)
C(33)-C(28)-P(2)	117.8(2)	C(48)-C(47)-H(47)	119.8
C(28)-C(29)-C(30)	121.1(3)	C(46)-C(47)-H(47)	119.8
C(28)-C(29)-H(29)	119.4	C(47)-C(48)-C(49)	121.5(3)
C(30)-C(29)-H(29)	119.4	C(47)-C(48)-H(48)	119.3
C(31)-C(30)-C(29)	120.0(3)	C(49)-C(48)-H(48)	119.3
C(31)-C(30)-H(30)	120.0	C(50)-C(49)-C(48)	118.2(2)
C(29)-C(30)-H(30)	120.0	C(50)-C(49)-C(52)	121.7(3)
C(30)-C(31)-C(32)	119.9(3)	C(48)-C(49)-C(52)	120.0(3)
C(30)-C(31)-H(31)	120.0	C(51)-C(50)-C(49)	120.9(3)

C(51)-C(50)-H(50)	119.5	C(58)-C(57)-H(57)	119.7
C(49)-C(50)-H(50)	119.5	C(57)-C(58)-C(53)	122.9(2)
C(50)-C(51)-C(46)	121.1(2)	C(57)-C(58)-H(58)	118.6
C(50)-C(51)-H(51)	119.5	C(53)-C(58)-H(58)	118.6
C(46)-C(51)-H(51)	119.5	B(2)-C(59)-P(4)	115.90(16)
C(49)-C(52)-H(52A)	109.5	B(2)-C(59)-H(59A)	108.3
C(49)-C(52)-H(52B)	109.5	P(4)-C(59)-H(59A)	108.3
H(52A)-C(52)-H(52B)	109.5	B(2)-C(59)-H(59B)	108.3
C(49)-C(52)-H(52C)	109.5	P(4)-C(59)-H(59B)	108.3
H(52A)-C(52)-H(52C)	109.5	H(59A)-C(59)-H(59B)	107.4
H(52B)-C(52)-H(52C)	109.5	B(2)-C(60)-P(5)	116.33(16)
N(2)-Fe(2)-P(5)	107.62(7)	B(2)-C(60)-H(60A)	108.2
N(2)-Fe(2)-P(4)	130.71(7)	P(5)-C(60)-H(60A)	108.2
P(5)-Fe(2)-P(4)	88.18(3)	B(2)-C(60)-H(60B)	108.2
N(2)-Fe(2)-P(6)	133.84(7)	P(5)-C(60)-H(60B)	108.2
P(5)-Fe(2)-P(6)	90.41(3)	H(60A)-C(60)-H(60B)	107.4
P(4)-Fe(2)-P(6)	90.79(3)	B(2)-C(61)-P(6)	114.82(16)
C(99)-N(2)-Fe(2)	167.30(17)	B(2)-C(61)-H(61A)	108.6
C(59)-P(4)-C(68)	107.31(11)	P(6)-C(61)-H(61A)	108.6
C(59)-P(4)-C(62)	107.25(11)	B(2)-C(61)-H(61B)	108.6
C(68)-P(4)-C(62)	100.82(11)	P(6)-C(61)-H(61B)	108.6
C(59)-P(4)-Fe(2)	116.06(8)	H(61A)-C(61)-H(61B)	107.5
C(68)-P(4)-Fe(2)	111.75(8)	C(63)-C(62)-C(67)	118.6(2)
C(62)-P(4)-Fe(2)	112.44(8)	C(63)-C(62)-P(4)	120.68(19)
C(60)-P(5)-C(80)	108.15(11)	C(67)-C(62)-P(4)	120.72(19)
C(60)-P(5)-C(74)	104.98(11)	C(62)-C(63)-C(64)	120.5(2)
C(80)-P(5)-C(74)	100.86(10)	C(62)-C(63)-H(63)	119.8
C(60)-P(5)-Fe(2)	116.93(8)	C(64)-C(63)-H(63)	119.8
C(80)-P(5)-Fe(2)	108.48(7)	C(65)-C(64)-C(63)	119.8(3)
C(74)-P(5)-Fe(2)	116.06(8)	C(65)-C(64)-H(64)	120.1
C(61)-P(6)-C(86)	106.78(11)	C(63)-C(64)-H(64)	120.1
C(61)-P(6)-C(92)	104.70(11)	C(64)-C(65)-C(66)	120.5(2)
C(86)-P(6)-C(92)	101.84(10)	C(64)-C(65)-H(65)	119.8
C(61)-P(6)-Fe(2)	116.47(8)	C(66)-C(65)-H(65)	119.8
C(86)-P(6)-Fe(2)	115.23(8)	C(65)-C(66)-C(67)	119.9(2)
C(92)-P(6)-Fe(2)	110.35(8)	C(65)-C(66)-H(66)	120.1
C(53)-B(2)-C(60)	111.43(19)	C(67)-C(66)-H(66)	120.1
C(53)-B(2)-C(61)	107.43(19)	C(66)-C(67)-C(62)	120.8(2)
C(60)-B(2)-C(61)	107.46(19)	C(66)-C(67)-H(67)	119.6
C(53)-B(2)-C(59)	107.89(19)	C(62)-C(67)-H(67)	119.6
C(60)-B(2)-C(59)	109.78(19)	C(73)-C(68)-C(69)	118.3(2)
C(61)-B(2)-C(59)	112.87(19)	C(73)-C(68)-P(4)	123.21(19)
C(58)-C(53)-C(54)	114.5(2)	C(69)-C(68)-P(4)	118.43(19)
C(58)-C(53)-B(2)	124.7(2)	C(70)-C(69)-C(68)	120.7(2)
C(54)-C(53)-B(2)	120.7(2)	C(70)-C(69)-H(69)	119.6
C(55)-C(54)-C(53)	123.0(2)	C(68)-C(69)-H(69)	119.6
C(55)-C(54)-H(54)	118.5	C(71)-C(70)-C(69)	120.1(3)
C(53)-C(54)-H(54)	118.5	C(71)-C(70)-H(70)	119.9
C(56)-C(55)-C(54)	120.0(3)	C(69)-C(70)-H(70)	119.9
C(56)-C(55)-H(55)	120.0	C(72)-C(71)-C(70)	120.3(3)
C(54)-C(55)-H(55)	120.0	C(72)-C(71)-H(71)	119.9
C(57)-C(56)-C(55)	118.9(2)	C(70)-C(71)-H(71)	119.9
C(57)-C(56)-H(56)	120.6	C(71)-C(72)-C(73)	119.8(3)
C(55)-C(56)-H(56)	120.6	C(71)-C(72)-H(72)	120.1
C(56)-C(57)-C(58)	120.7(3)	C(73)-C(72)-H(72)	120.1
C(56)-C(57)-H(57)	119.7	C(68)-C(73)-C(72)	120.9(2)

C(68)-C(73)-H(73)	119.6	C(97)-C(92)-C(93)	118.2(2)
C(72)-C(73)-H(73)	119.6	C(97)-C(92)-P(6)	122.85(19)
C(75)-C(74)-C(79)	118.6(2)	C(93)-C(92)-P(6)	118.96(19)
C(75)-C(74)-P(5)	122.00(18)	C(94)-C(93)-C(92)	120.8(2)
C(79)-C(74)-P(5)	119.34(19)	C(94)-C(93)-H(93)	119.6
C(74)-C(75)-C(76)	120.4(2)	C(92)-C(93)-H(93)	119.6
C(74)-C(75)-H(75)	119.8	C(95)-C(94)-C(93)	120.1(2)
C(76)-C(75)-H(75)	119.8	C(95)-C(94)-H(94)	120.0
C(77)-C(76)-C(75)	120.3(3)	C(93)-C(94)-H(94)	120.0
C(77)-C(76)-H(76)	119.9	C(96)-C(95)-C(94)	119.7(2)
C(75)-C(76)-H(76)	119.9	C(96)-C(95)-H(95)	120.2
C(78)-C(77)-C(76)	119.5(2)	C(94)-C(95)-H(95)	120.2
C(78)-C(77)-H(77)	120.3	C(95)-C(96)-C(97)	120.0(2)
C(76)-C(77)-H(77)	120.3	C(95)-C(96)-H(96)	120.0
C(79)-C(78)-C(77)	120.5(2)	C(97)-C(96)-H(96)	120.0
C(79)-C(78)-H(78)	119.8	C(92)-C(97)-C(96)	121.1(2)
C(77)-C(78)-H(78)	119.8	C(92)-C(97)-H(97)	119.4
C(78)-C(79)-C(74)	120.7(2)	C(96)-C(97)-H(97)	119.4
C(78)-C(79)-H(79)	119.7	C(102)-C(98)-H(98A)	109.5
C(74)-C(79)-H(79)	119.7	C(102)-C(98)-H(98B)	109.5
C(85)-C(80)-C(81)	118.4(2)	H(98A)-C(98)-H(98B)	109.5
C(85)-C(80)-P(5)	123.88(19)	C(102)-C(98)-H(98C)	109.5
C(81)-C(80)-P(5)	117.57(18)	H(98A)-C(98)-H(98C)	109.5
C(82)-C(81)-C(80)	120.7(2)	H(98B)-C(98)-H(98C)	109.5
C(82)-C(81)-H(81)	119.7	N(2)-C(99)-C(104)	121.5(2)
C(80)-C(81)-H(81)	119.7	N(2)-C(99)-C(100)	120.5(2)
C(81)-C(82)-C(83)	120.3(2)	C(104)-C(99)-C(100)	118.0(2)
C(81)-C(82)-H(82)	119.8	C(101)-C(100)-C(99)	120.7(2)
C(83)-C(82)-H(82)	119.8	C(101)-C(100)-H(100)	119.7
C(84)-C(83)-C(82)	119.4(2)	C(99)-C(100)-H(100)	119.7
C(84)-C(83)-H(83)	120.3	C(100)-C(101)-C(102)	121.3(2)
C(82)-C(83)-H(83)	120.3	C(100)-C(101)-H(101)	119.3
C(83)-C(84)-C(85)	120.1(2)	C(102)-C(101)-H(101)	119.3
C(83)-C(84)-H(84)	119.9	C(103)-C(102)-C(101)	118.0(2)
C(85)-C(84)-H(84)	119.9	C(103)-C(102)-C(98)	121.3(2)
C(80)-C(85)-C(84)	121.0(2)	C(101)-C(102)-C(98)	120.8(2)
C(80)-C(85)-H(85)	119.5	C(102)-C(103)-C(104)	121.2(2)
C(84)-C(85)-H(85)	119.5	C(102)-C(103)-H(103)	119.4
C(87)-C(86)-C(91)	118.2(2)	C(104)-C(103)-H(103)	119.4
C(87)-C(86)-P(6)	121.78(19)	C(103)-C(104)-C(99)	120.8(2)
C(91)-C(86)-P(6)	119.97(19)	C(103)-C(104)-H(104)	119.6
C(86)-C(87)-C(88)	120.5(2)	C(99)-C(104)-H(104)	119.6
C(86)-C(87)-H(87)	119.7	C(113)-C(108)-C(109)	123(2)
C(88)-C(87)-H(87)	119.7	C(113)-C(108)-H(108)	118.5
C(89)-C(88)-C(87)	120.4(2)	C(109)-C(108)-H(108)	118.6
C(89)-C(88)-H(88)	119.8	C(113)-C(108)-H(119)	81.2
C(87)-C(88)-H(88)	119.8	C(109)-C(108)-H(119)	144.5
C(90)-C(89)-C(88)	119.7(2)	H(108)-C(108)-H(119)	46.3
C(90)-C(89)-H(89)	120.1	C(110)-C(109)-C(108)	109(2)
C(88)-C(89)-H(89)	120.1	C(110)-C(109)-H(109)	125.5
C(89)-C(90)-C(91)	120.6(3)	C(108)-C(109)-H(109)	125.5
C(89)-C(90)-H(90)	119.7	C(112)-C(111)-C(110)	119(2)
C(91)-C(90)-H(90)	119.7	C(112)-C(111)-H(111)	120.6
C(90)-C(91)-C(86)	120.6(2)	C(110)-C(111)-H(111)	120.6
C(90)-C(91)-H(91)	119.7	C(111)-C(112)-C(113)	125(2)
C(86)-C(91)-H(91)	119.7	C(111)-C(112)-H(112)	117.4

C(113)-C(112)-H(112)	117.4	C(115)-C(114)-H(114)	116.5
C(112)-C(113)-C(108)	121.6(18)	C(117)-C(116)-C(115)	122.2(14)
C(112)-C(113)-H(113)	119.2	C(117)-C(116)-H(116)	118.9
C(108)-C(113)-H(113)	119.2	C(115)-C(116)-H(116)	118.9
C(112)-C(113)-H(119)	149.7	C(116)-C(117)-C(118)	123.7(17)
C(108)-C(113)-H(119)	31.9	C(116)-C(117)-H(117)	118.2
H(113)-C(113)-H(119)	89.1	C(118)-C(117)-H(117)	118.2
C(109)-C(110)-C(111)	122(2)	C(117)-C(118)-C(119)	115.9(19)
C(109)-C(110)-H(110)	119.0	C(117)-C(118)-H(118)	122.0
C(111)-C(110)-H(110)	119.0	C(119)-C(118)-H(118)	122.0
C(114)-C(119)-C(118)	118.5(14)	C(114)-C(115)-C(116)	112.3(11)
C(114)-C(119)-H(119)	121.0	C(114)-C(115)-H(115)	123.8
C(118)-C(119)-H(119)	120.5	C(116)-C(115)-H(115)	123.8
C(119)-C(114)-C(115)	127.0(12)		
C(119)-C(114)-H(114)	116.5		

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[PhBP_3]FeNTol \cdot C_6H_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	17(1)	16(1)	20(1)	-1(1)	-3(1)	-3(1)
P(1)	16(1)	16(1)	18(1)	-2(1)	-1(1)	-3(1)
P(2)	16(1)	17(1)	20(1)	0(1)	0(1)	-3(1)
P(3)	16(1)	17(1)	23(1)	-1(1)	-1(1)	-4(1)
N(1)	18(1)	19(1)	22(1)	-1(1)	0(1)	-5(1)
B(1)	17(2)	17(2)	21(2)	-2(1)	-1(1)	-4(1)
C(1)	23(1)	11(1)	25(1)	-5(1)	-3(1)	0(1)
C(2)	26(2)	20(1)	25(2)	0(1)	-3(1)	-4(1)
C(3)	40(2)	23(2)	24(2)	3(1)	-4(1)	-5(1)
C(4)	45(2)	24(2)	25(2)	-1(1)	-17(1)	-5(1)
C(5)	33(2)	27(2)	34(2)	-1(1)	-14(1)	-11(1)
C(6)	28(2)	22(2)	24(2)	-1(1)	-5(1)	-7(1)
C(7)	22(1)	18(1)	17(1)	2(1)	-2(1)	-4(1)
C(8)	18(1)	20(1)	23(1)	-4(1)	-2(1)	-5(1)
C(9)	20(1)	16(1)	20(1)	-2(1)	-1(1)	-4(1)
C(10)	14(1)	18(1)	24(1)	3(1)	1(1)	-2(1)
C(11)	22(2)	29(2)	31(2)	0(1)	-3(1)	-6(1)
C(12)	17(2)	38(2)	52(2)	6(2)	-4(1)	-9(1)
C(13)	21(2)	39(2)	42(2)	9(2)	10(1)	-3(1)
C(14)	30(2)	40(2)	25(2)	4(1)	7(1)	-4(1)
C(15)	20(2)	31(2)	25(2)	3(1)	-2(1)	-4(1)
C(16)	15(1)	16(1)	20(1)	-3(1)	3(1)	-3(1)
C(17)	21(1)	21(1)	24(2)	-2(1)	-6(1)	-3(1)
C(18)	21(2)	24(2)	32(2)	-7(1)	-5(1)	-7(1)
C(19)	24(2)	16(1)	32(2)	-5(1)	-1(1)	-4(1)
C(20)	30(2)	19(1)	23(2)	1(1)	-6(1)	-2(1)
C(21)	22(1)	21(1)	20(1)	-4(1)	-4(1)	-5(1)
C(22)	17(1)	16(1)	22(1)	0(1)	-1(1)	-2(1)
C(23)	33(2)	28(2)	23(2)	-7(1)	4(1)	-10(1)
C(24)	29(2)	28(2)	37(2)	-4(1)	3(1)	-16(1)
C(25)	24(2)	33(2)	21(2)	7(1)	2(1)	-8(1)
C(26)	29(2)	34(2)	21(2)	-2(1)	2(1)	-11(1)
C(27)	26(2)	28(2)	27(2)	0(1)	0(1)	-11(1)
C(28)	14(1)	17(1)	30(2)	3(1)	3(1)	-5(1)
C(29)	26(2)	21(2)	31(2)	-2(1)	5(1)	-5(1)
C(30)	39(2)	21(2)	42(2)	-4(1)	16(2)	-4(1)
C(31)	28(2)	17(2)	60(2)	2(2)	15(2)	-1(1)
C(32)	25(2)	28(2)	59(2)	10(2)	-9(2)	-7(1)
C(33)	25(2)	20(2)	36(2)	1(1)	-5(1)	-6(1)
C(34)	18(1)	14(1)	29(2)	1(1)	0(1)	-5(1)
C(35)	23(2)	30(2)	33(2)	1(1)	0(1)	0(1)
C(36)	23(2)	41(2)	44(2)	6(2)	-6(1)	0(1)
C(37)	19(2)	22(2)	69(2)	2(2)	2(2)	-2(1)
C(38)	23(2)	35(2)	64(2)	-23(2)	8(2)	-4(1)
C(39)	21(2)	37(2)	47(2)	-16(2)	5(1)	-7(1)
C(40)	12(1)	20(1)	24(1)	-1(1)	3(1)	-3(1)
C(41)	30(2)	32(2)	30(2)	4(1)	-6(1)	-14(1)
C(42)	38(2)	33(2)	37(2)	15(1)	-10(1)	-17(1)
C(43)	24(2)	23(2)	46(2)	5(1)	-2(1)	-10(1)
C(44)	28(2)	27(2)	33(2)	-3(1)	-1(1)	-14(1)

C(45)	24(2)	25(2)	26(2)	3(1)	-2(1)	-7(1)
C(46)	18(1)	24(2)	20(1)	4(1)	-2(1)	-9(1)
C(47)	30(2)	22(2)	27(2)	0(1)	-6(1)	-7(1)
C(48)	26(2)	26(2)	30(2)	7(1)	-9(1)	-4(1)
C(49)	24(2)	39(2)	19(1)	8(1)	-3(1)	-13(1)
C(50)	25(2)	39(2)	20(2)	-4(1)	0(1)	-9(1)
C(51)	17(1)	29(2)	27(2)	-3(1)	0(1)	-2(1)
C(52)	32(2)	50(2)	27(2)	2(1)	-7(1)	-13(2)
Fe(2)	14(1)	15(1)	19(1)	0(1)	-1(1)	-4(1)
N(2)	18(1)	17(1)	20(1)	1(1)	1(1)	-2(1)
P(4)	14(1)	16(1)	19(1)	-1(1)	0(1)	-4(1)
P(5)	13(1)	15(1)	20(1)	1(1)	-1(1)	-3(1)
P(6)	14(1)	15(1)	19(1)	1(1)	-1(1)	-3(1)
B(2)	12(1)	17(2)	18(2)	0(1)	-1(1)	-1(1)
C(53)	11(1)	17(1)	24(1)	-4(1)	0(1)	2(1)
C(54)	18(1)	27(2)	28(2)	-6(1)	1(1)	-2(1)
C(55)	19(2)	22(2)	43(2)	-9(1)	-9(1)	-1(1)
C(56)	36(2)	23(2)	32(2)	-10(1)	-19(1)	4(1)
C(57)	53(2)	25(2)	23(2)	-3(1)	-9(1)	-3(2)
C(58)	30(2)	18(1)	26(2)	-4(1)	-3(1)	-4(1)
C(59)	16(1)	16(1)	23(1)	-3(1)	-2(1)	-4(1)
C(60)	12(1)	21(1)	18(1)	-1(1)	-3(1)	0(1)
C(61)	16(1)	20(1)	17(1)	-2(1)	-2(1)	-5(1)
C(62)	18(1)	14(1)	20(1)	0(1)	3(1)	-4(1)
C(63)	21(2)	33(2)	29(2)	-1(1)	1(1)	-8(1)
C(64)	28(2)	39(2)	25(2)	9(1)	-3(1)	-9(1)
C(65)	28(2)	30(2)	28(2)	5(1)	9(1)	-9(1)
C(66)	19(2)	27(2)	37(2)	0(1)	5(1)	-8(1)
C(67)	19(1)	21(1)	26(2)	-1(1)	0(1)	-5(1)
C(68)	11(1)	16(1)	27(1)	-2(1)	3(1)	-5(1)
C(69)	20(1)	22(1)	31(2)	-2(1)	-1(1)	-9(1)
C(70)	26(2)	25(2)	42(2)	-14(1)	7(1)	-10(1)
C(71)	26(2)	17(2)	58(2)	-2(2)	8(2)	-2(1)
C(72)	23(2)	26(2)	45(2)	11(1)	1(1)	-1(1)
C(73)	17(1)	24(2)	26(2)	-1(1)	1(1)	-3(1)
C(74)	10(1)	16(1)	26(1)	3(1)	-1(1)	-3(1)
C(75)	20(1)	23(2)	25(2)	2(1)	-4(1)	-8(1)
C(76)	33(2)	22(2)	35(2)	-8(1)	-1(1)	-7(1)
C(77)	28(2)	15(1)	47(2)	1(1)	-1(1)	-4(1)
C(78)	25(2)	23(2)	33(2)	10(1)	0(1)	-1(1)
C(79)	21(2)	22(2)	26(2)	-2(1)	2(1)	-2(1)
C(80)	14(1)	16(1)	18(1)	8(1)	-2(1)	-2(1)
C(81)	21(2)	18(1)	27(2)	4(1)	-3(1)	-3(1)
C(82)	15(1)	26(2)	34(2)	4(1)	-6(1)	-8(1)
C(83)	14(1)	31(2)	32(2)	9(1)	1(1)	-3(1)
C(84)	22(2)	26(2)	26(2)	-1(1)	5(1)	0(1)
C(85)	20(1)	22(1)	21(1)	1(1)	-2(1)	-6(1)
C(86)	16(1)	16(1)	16(1)	2(1)	0(1)	-1(1)
C(87)	24(2)	19(1)	28(2)	1(1)	-5(1)	-4(1)
C(88)	17(1)	29(2)	36(2)	1(1)	-6(1)	-6(1)
C(89)	18(1)	34(2)	27(2)	0(1)	-1(1)	7(1)
C(90)	29(2)	31(2)	36(2)	-14(1)	-8(1)	8(1)
C(91)	21(2)	27(2)	35(2)	-7(1)	-10(1)	-2(1)
C(92)	15(1)	14(1)	22(1)	-1(1)	3(1)	-1(1)
C(93)	23(2)	29(2)	25(2)	0(1)	-2(1)	-9(1)
C(94)	32(2)	36(2)	24(2)	8(1)	-4(1)	-9(1)

C(95)	28(2)	22(2)	34(2)	8(1)	7(1)	-7(1)
C(96)	23(2)	23(2)	37(2)	-2(1)	2(1)	-9(1)
C(97)	25(2)	19(1)	23(1)	-1(1)	-3(1)	-6(1)
C(98)	38(2)	39(2)	29(2)	-1(1)	-7(1)	-19(2)
C(99)	22(1)	17(1)	19(1)	5(1)	-5(1)	-7(1)
C(100)	22(2)	27(2)	24(2)	-2(1)	-1(1)	-8(1)
C(101)	33(2)	25(2)	21(2)	-4(1)	-1(1)	-6(1)
C(102)	32(2)	25(2)	22(2)	3(1)	-7(1)	-14(1)
C(103)	21(2)	28(2)	28(2)	2(1)	-2(1)	-10(1)
C(104)	21(1)	21(1)	22(1)	-1(1)	0(1)	-4(1)
C(108)	23(8)	40(7)	53(9)	-14(6)	19(6)	-4(7)
C(109)	68(16)	103(15)	65(18)	-36(10)	20(12)	-69(11)
C(111)	28(9)	100(20)	23(8)	13(10)	13(7)	-5(9)
C(112)	78(15)	48(11)	53(10)	12(10)	41(10)	5(11)
C(113)	53(10)	39(7)	33(7)	-14(6)	15(6)	-19(7)
C(110)	54(13)	75(16)	41(7)	14(12)	-11(8)	-34(13)
C(119)	25(7)	119(15)	28(5)	-6(7)	10(4)	-6(8)
C(114)	24(5)	33(5)	32(5)	-7(4)	1(4)	-2(5)
C(116)	43(5)	51(7)	48(6)	13(4)	-1(4)	17(4)
C(117)	110(20)	44(11)	115(16)	9(10)	36(14)	34(11)
C(118)	75(15)	76(14)	67(13)	-28(12)	29(10)	-47(12)
C(115)	36(5)	52(6)	59(5)	1(5)	11(4)	-10(5)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]FeNTol \cdot C_6H_6$.

	x	y	z	U(eq)
H(2)	569	8285	1812	28
H(3)	-394	8219	1042	35
H(4)	-2190	7677	1071	37
H(5)	-2972	7173	1890	36
H(6)	-1990	7230	2660	29
H(7A)	-1424	8965	2987	23
H(7B)	-103	9177	2785	23
H(8A)	-305	6685	3222	24
H(8B)	-1255	7425	3490	24
H(9A)	1821	7976	2452	23
H(9B)	1933	7096	2757	23
H(11)	-2737	8646	3567	33
H(12)	-4578	8719	4112	43
H(13)	-4700	9128	4969	43
H(14)	-2955	9463	5294	40
H(15)	-1087	9359	4765	31
H(17)	924	9968	4325	26
H(18)	935	11345	4338	30
H(19)	-154	12288	3716	29
H(20)	-1266	11860	3092	29
H(21)	-1300	10489	3077	25
H(23)	-900	5843	4118	33
H(24)	-1973	5312	4848	36
H(25)	-2092	5851	5669	32
H(26)	-1138	6930	5762	33
H(27)	-17	7444	5036	32
H(29)	1371	5851	3132	31
H(30)	3107	4786	2999	42
H(31)	4644	4455	3615	44
H(32)	4402	5150	4386	45
H(33)	2657	6215	4525	32
H(35)	4329	7663	4036	36
H(36)	6375	6881	4070	45
H(37)	7224	6050	3379	45
H(38)	6080	6078	2638	49
H(39)	4054	6891	2599	41
H(41)	2127	9171	2358	36
H(42)	2439	10494	2187	42
H(43)	3185	11126	2835	37
H(44)	3707	10417	3649	34
H(45)	3336	9116	3831	30
H(47)	4093	6879	4847	31
H(48)	5585	6807	5460	33
H(50)	3662	8928	6014	33
H(51)	2154	9011	5405	30
H(52A)	6263	7280	6237	54
H(52B)	5508	8116	6470	54
H(52C)	6474	8132	5961	54
H(54)	8493	4595	2457	29
H(55)	9442	4956	3161	33

H(56)	9045	4426	4026	37
H(57)	7691	3537	4170	41
H(58)	6776	3154	3467	30
H(59A)	8755	3059	2002	22
H(59B)	8216	3956	1748	22
H(60A)	5785	2821	2837	21
H(60B)	7046	2287	2575	21
H(61A)	5943	4860	2235	21
H(61B)	4990	4322	2494	21
H(63)	6920	3555	207	33
H(64)	7941	4078	-548	37
H(65)	9953	4290	-505	35
H(66)	10962	3993	286	33
H(67)	9976	3444	1034	26
H(69)	8213	1832	507	28
H(70)	9181	459	493	36
H(71)	9974	-266	1263	42
H(72)	9844	384	2044	40
H(73)	8890	1769	2060	27
H(75)	5913	1238	1226	27
H(76)	6445	-183	1279	35
H(77)	6710	-911	2104	36
H(78)	6408	-215	2876	34
H(79)	5902	1195	2827	29
H(81)	3315	1931	1718	27
H(82)	1172	2172	1962	29
H(83)	329	3010	2651	32
H(84)	1646	3623	3082	31
H(85)	3789	3398	2827	25
H(87)	2708	3918	1368	28
H(88)	588	4566	1466	32
H(89)	3	5855	1782	34
H(90)	1536	6510	1990	40
H(91)	3653	5873	1905	33
H(93)	4589	5131	545	31
H(94)	5372	6099	-9	37
H(95)	7040	6607	244	34
H(96)	7905	6150	1056	32
H(97)	7074	5216	1625	26
H(98A)	1408	662	14	50
H(98B)	2740	99	-159	50
H(98C)	2102	850	-549	50
H(100)	5683	1583	137	28
H(101)	4643	762	-260	32
H(103)	1357	1836	485	30
H(104)	2383	2676	877	26
H(108)	8562	975	9361	48
H(109)	7105	217	8925	84
H(111)	5148	2681	8562	63
H(112)	6373	3130	9029	79
H(113)	7978	2335	9455	48
H(110)	5531	1156	8444	65
H(119)	8129	1296	9471	72
H(114)	7697	311	9085	36
H(116)	4932	1832	8330	63
H(117)	5548	2844	8609	120

H(118)	7170	2671	9177	82
H(115)	5977	455	8556	60

Table 16. Crystal data and structure refinement for $[PhBP_3]Fe(CO)_2$.

Identification code	sdb18	
Empirical formula	$C_{47}H_{41}BFeO_2P_3$	
Formula weight	797.37	
Crystal Habit	blades	
Crystal Color	dichroic	
Crystal size	0.074 x 0.22 x 0.56 mm^3	
Type of diffractometer	Bruker P4	
Wavelength	0.71073 Å	
Data collection temperature	98(2) K	
Unit cell dimensions	a = 9.7323(9) Å	α= 90°.
	b = 17.2050(15) Å	β= 95.718(2)°.
	c = 23.208(2) Å	γ = 90°.
Volume	3866.8(6) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Density (calculated)	1.370 Mg/m^3	
F(000)	1660	
Theta range for data collection	1.48 to 28.49°.	
Completeness to theta = 28.49°	89.8 %	
Index ranges	-12<=h<=12, -20<=k<=22, -28<=l<=30	
Reflections collected	23586	
Independent reflections	8782 [R(int) = 0.0618]	
Absorption coefficient	0.554 mm^{-1}	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8782 / 0 / 524	
Goodness-of-fit on F^2	1.189	
Final R indices [I>2sigma(I)]	R1 = 0.0503, wR2 = 0.0886	
R indices (all data)	R1 = 0.0861, wR2 = 0.0955	
Largest diff. peak and hole	0.752 and -0.541 $e.Å^{-3}$	

Special Refinement Details

One phenyl ring off of P3 within the [$PhBP_3$] ligand has two orientations with four carbons being split between the two positions (C37-C38-C39-C34). Refining the population density between the positions reveals that the crystal has an almost equal population (51%) of the two conformations within the lattice.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]Fe(CO)_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3835(1)	7433(1)	1990(1)	19(1)
P(1)	1468(1)	7403(1)	2014(1)	18(1)
P(2)	3932(1)	6252(1)	2440(1)	18(1)
P(3)	3568(1)	6957(1)	1077(1)	20(1)
O(1)	3981(2)	9078(1)	1736(1)	48(1)
O(2)	6821(2)	7620(1)	2045(1)	40(1)
B	1657(3)	5842(2)	1558(1)	19(1)
C(1)	746(3)	5062(2)	1377(1)	19(1)
C(2)	607(3)	4734(2)	822(1)	24(1)
C(3)	-112(3)	4051(2)	695(1)	26(1)
C(4)	-757(3)	3669(2)	1115(1)	27(1)
C(5)	-655(3)	3975(2)	1667(1)	25(1)
C(6)	77(3)	4651(2)	1792(1)	22(1)
C(7)	757(3)	6432(2)	1942(1)	20(1)
C(8)	3038(3)	5534(2)	1983(1)	18(1)
C(9)	2129(3)	6279(2)	968(1)	26(1)
C(10)	460(3)	7992(2)	1457(1)	23(1)
C(11)	667(3)	8783(2)	1442(1)	30(1)
C(12)	-60(3)	9249(2)	1034(1)	36(1)
C(13)	-1031(3)	8921(2)	636(1)	39(1)
C(14)	-1291(3)	8135(2)	654(1)	35(1)
C(15)	-542(3)	7671(2)	1062(1)	28(1)
C(16)	897(3)	7830(2)	2671(1)	19(1)
C(17)	-357(3)	7619(2)	2851(1)	28(1)
C(18)	-831(3)	7951(2)	3337(1)	31(1)
C(19)	-46(3)	8490(2)	3652(1)	27(1)
C(20)	1226(3)	8700(2)	3485(1)	25(1)
C(21)	1691(3)	8373(2)	2996(1)	21(1)
C(22)	3172(3)	6297(2)	3131(1)	18(1)
C(23)	2303(3)	5738(2)	3314(1)	22(1)
C(24)	1773(3)	5807(2)	3846(1)	29(1)
C(25)	2104(3)	6438(2)	4193(1)	31(1)
C(26)	2990(3)	6999(2)	4021(1)	28(1)
C(27)	3518(3)	6931(2)	3492(1)	23(1)
C(28)	5614(3)	5828(2)	2697(1)	20(1)
C(29)	5909(3)	5054(2)	2596(1)	27(1)
C(30)	7144(3)	4726(2)	2823(1)	34(1)
C(31)	8103(3)	5171(2)	3152(1)	32(1)
C(32)	7833(3)	5939(2)	3252(1)	30(1)
C(33)	6596(3)	6263(2)	3032(1)	26(1)
C(35)	6007(3)	6065(2)	1183(1)	23(1)
C(36)	7057(3)	5621(2)	998(1)	33(1)
C(40)	3343(3)	7728(2)	532(1)	23(1)
C(41)	2171(3)	7829(2)	148(1)	27(1)
C(42)	2053(3)	8458(2)	-226(1)	35(1)
C(43)	3099(4)	8996(2)	-222(1)	38(1)
C(44)	4279(4)	8898(2)	154(1)	43(1)
C(45)	4394(3)	8275(2)	525(1)	38(1)
C(46)	3840(3)	8428(2)	1836(1)	31(1)
C(47)	5654(3)	7516(2)	2039(1)	26(1)
C(34A)	5160(12)	6525(6)	825(6)	12(2)

C(37A)	7483(6)	5789(4)	450(2)	25(1)
C(38A)	6673(6)	6261(3)	79(2)	29(2)
C(39A)	5505(5)	6611(3)	258(2)	21(1)
C(34B)	4836(15)	6296(7)	815(7)	21(2)
C(37B)	6729(6)	5262(4)	431(3)	30(2)
C(38B)	5574(6)	5467(4)	76(3)	31(2)
C(39B)	4642(6)	5985(4)	270(2)	28(2)

Table 18. Bond lengths [Å] and angles [°] for $[PhBP_3]Fe(CO)_2$.

Fe(1)-C(46)	1.750(3)	C(18)-H(18)	0.9500
Fe(1)-C(47)	1.769(3)	C(19)-C(20)	1.381(4)
Fe(1)-P(3)	2.2626(8)	C(19)-H(19)	0.9500
Fe(1)-P(2)	2.2819(8)	C(20)-C(21)	1.383(3)
Fe(1)-P(1)	2.3104(8)	C(20)-H(20)	0.9500
P(1)-C(7)	1.809(3)	C(21)-H(21)	0.9500
P(1)-C(16)	1.828(3)	C(22)-C(23)	1.375(4)
P(1)-C(10)	1.847(3)	C(22)-C(27)	1.395(4)
P(2)-C(8)	1.795(3)	C(23)-C(24)	1.390(4)
P(2)-C(22)	1.835(3)	C(23)-H(23)	0.9500
P(2)-C(28)	1.837(3)	C(24)-C(25)	1.369(4)
P(3)-C(9)	1.820(3)	C(24)-H(24)	0.9500
P(3)-C(34B)	1.826(16)	C(25)-C(26)	1.381(4)
P(3)-C(40)	1.831(3)	C(25)-H(25)	0.9500
P(3)-C(34A)	1.864(14)	C(26)-C(27)	1.381(4)
O(1)-C(46)	1.153(3)	C(26)-H(26)	0.9500
O(2)-C(47)	1.148(3)	C(27)-H(27)	0.9500
B-C(1)	1.639(4)	C(28)-C(29)	1.386(4)
B-C(7)	1.658(4)	C(28)-C(33)	1.389(4)
B-C(9)	1.665(4)	C(29)-C(30)	1.384(4)
B-C(8)	1.672(4)	C(29)-H(29)	0.9500
C(1)-C(2)	1.400(3)	C(30)-C(31)	1.377(4)
C(1)-C(6)	1.407(4)	C(30)-H(30)	0.9500
C(2)-C(3)	1.383(4)	C(31)-C(32)	1.371(4)
C(2)-H(2)	0.9500	C(31)-H(31)	0.9500
C(3)-C(4)	1.377(4)	C(32)-C(33)	1.379(4)
C(3)-H(3)	0.9500	C(32)-H(32)	0.9500
C(4)-C(5)	1.380(4)	C(33)-H(33)	0.9500
C(4)-H(4)	0.9500	C(35)-C(34A)	1.365(14)
C(5)-C(6)	1.380(4)	C(35)-C(36)	1.378(4)
C(5)-H(5)	0.9500	C(35)-C(34B)	1.412(17)
C(6)-H(6)	0.9500	C(35)-H(35)	0.9500
C(7)-H(7A)	0.9900	C(36)-C(37A)	1.407(6)
C(7)-H(7B)	0.9900	C(36)-C(37B)	1.460(7)
C(8)-H(8A)	0.9900	C(36)-H(36)	0.9500
C(8)-H(8B)	0.9900	C(40)-C(41)	1.387(4)
C(9)-H(9A)	0.9900	C(40)-C(45)	1.391(4)
C(9)-H(9B)	0.9900	C(41)-C(42)	1.385(4)
C(10)-C(11)	1.375(4)	C(41)-H(41)	0.9500
C(10)-C(15)	1.386(4)	C(42)-C(43)	1.376(4)
C(11)-C(12)	1.382(4)	C(42)-H(42)	0.9500
C(11)-H(11)	0.9500	C(43)-C(44)	1.382(4)
C(12)-C(13)	1.375(4)	C(43)-H(43)	0.9500
C(12)-H(12)	0.9500	C(44)-C(45)	1.372(4)
C(13)-C(14)	1.377(4)	C(44)-H(44)	0.9500
C(13)-H(13)	0.9500	C(45)-H(45)	0.9500
C(14)-C(15)	1.389(4)	C(34A)-C(39A)	1.398(14)
C(14)-H(14)	0.9500	C(37A)-C(38A)	1.372(7)
C(15)-H(15)	0.9500	C(37A)-H(37A)	0.9500
C(16)-C(17)	1.377(4)	C(38A)-C(39A)	1.386(7)
C(16)-C(21)	1.385(4)	C(38A)-H(38A)	0.9500
C(17)-C(18)	1.382(4)	C(39A)-H(39A)	0.9500
C(17)-H(17)	0.9500	C(34B)-C(39B)	1.369(16)
C(18)-C(19)	1.367(4)	C(37B)-C(38B)	1.372(8)

C(37B)-H(37B)	0.9500	C(6)-C(5)-C(4)	120.4(3)
C(38B)-C(39B)	1.379(8)	C(6)-C(5)-H(5)	119.8
C(38B)-C(38B)#1	1.967(13)	C(4)-C(5)-H(5)	119.8
C(38B)-H(38B)	0.9500	C(5)-C(6)-C(1)	122.9(3)
C(39B)-H(39B)	0.9500	C(5)-C(6)-H(6)	118.5
		C(1)-C(6)-H(6)	118.5
C(46)-Fe(1)-C(47)	84.89(13)	B-C(7)-P(1)	113.47(18)
C(46)-Fe(1)-P(3)	99.49(10)	B-C(7)-H(7A)	108.9
C(47)-Fe(1)-P(3)	96.35(9)	P(1)-C(7)-H(7A)	108.9
C(46)-Fe(1)-P(2)	164.63(10)	B-C(7)-H(7B)	108.9
C(47)-Fe(1)-P(2)	92.69(9)	P(1)-C(7)-H(7B)	108.9
P(3)-Fe(1)-P(2)	95.86(3)	H(7A)-C(7)-H(7B)	107.7
C(46)-Fe(1)-P(1)	92.83(10)	B-C(8)-P(2)	116.42(18)
C(47)-Fe(1)-P(1)	173.88(9)	B-C(8)-H(8A)	108.2
P(3)-Fe(1)-P(1)	89.63(3)	P(2)-C(8)-H(8A)	108.2
P(2)-Fe(1)-P(1)	88.01(3)	B-C(8)-H(8B)	108.2
C(7)-P(1)-C(16)	107.68(12)	P(2)-C(8)-H(8B)	108.2
C(7)-P(1)-C(10)	105.64(12)	H(8A)-C(8)-H(8B)	107.3
C(16)-P(1)-C(10)	100.35(12)	B-C(9)-P(3)	116.58(18)
C(7)-P(1)-Fe(1)	113.00(9)	B-C(9)-H(9A)	108.1
C(16)-P(1)-Fe(1)	113.48(9)	P(3)-C(9)-H(9A)	108.1
C(10)-P(1)-Fe(1)	115.59(9)	B-C(9)-H(9B)	108.1
C(8)-P(2)-C(22)	109.40(12)	P(3)-C(9)-H(9B)	108.1
C(8)-P(2)-C(28)	106.41(12)	H(9A)-C(9)-H(9B)	107.3
C(22)-P(2)-C(28)	99.02(11)	C(11)-C(10)-C(15)	118.3(3)
C(8)-P(2)-Fe(1)	110.27(9)	C(11)-C(10)-P(1)	119.4(2)
C(22)-P(2)-Fe(1)	111.14(9)	C(15)-C(10)-P(1)	122.3(2)
C(28)-P(2)-Fe(1)	119.82(9)	C(10)-C(11)-C(12)	121.6(3)
C(9)-P(3)-C(34B)	95.3(3)	C(10)-C(11)-H(11)	119.2
C(9)-P(3)-C(40)	109.36(13)	C(12)-C(11)-H(11)	119.2
C(34B)-P(3)-C(40)	105.0(5)	C(13)-C(12)-C(11)	119.6(3)
C(9)-P(3)-C(34A)	110.7(3)	C(13)-C(12)-H(12)	120.2
C(34B)-P(3)-C(34A)	15.6(3)	C(11)-C(12)-H(12)	120.2
C(40)-P(3)-C(34A)	96.8(4)	C(12)-C(13)-C(14)	119.9(3)
C(9)-P(3)-Fe(1)	112.09(9)	C(12)-C(13)-H(13)	120.1
C(34B)-P(3)-Fe(1)	121.2(5)	C(14)-C(13)-H(13)	120.1
C(40)-P(3)-Fe(1)	112.28(9)	C(13)-C(14)-C(15)	120.0(3)
C(34A)-P(3)-Fe(1)	114.6(4)	C(13)-C(14)-H(14)	120.0
C(1)-B-C(7)	109.7(2)	C(15)-C(14)-H(14)	120.0
C(1)-B-C(9)	110.2(2)	C(10)-C(15)-C(14)	120.5(3)
C(7)-B-C(9)	111.6(2)	C(10)-C(15)-H(15)	119.7
C(1)-B-C(8)	105.9(2)	C(14)-C(15)-H(15)	119.7
C(7)-B-C(8)	108.2(2)	C(17)-C(16)-C(21)	118.4(2)
C(9)-B-C(8)	110.9(2)	C(17)-C(16)-P(1)	120.0(2)
C(2)-C(1)-C(6)	114.7(2)	C(21)-C(16)-P(1)	121.6(2)
C(2)-C(1)-B	124.5(2)	C(16)-C(17)-C(18)	121.1(3)
C(6)-C(1)-B	120.7(2)	C(16)-C(17)-H(17)	119.5
C(3)-C(2)-C(1)	122.6(3)	C(18)-C(17)-H(17)	119.5
C(3)-C(2)-H(2)	118.7	C(19)-C(18)-C(17)	120.2(3)
C(1)-C(2)-H(2)	118.7	C(19)-C(18)-H(18)	119.9
C(4)-C(3)-C(2)	120.8(3)	C(17)-C(18)-H(18)	119.9
C(4)-C(3)-H(3)	119.6	C(18)-C(19)-C(20)	119.7(3)
C(2)-C(3)-H(3)	119.6	C(18)-C(19)-H(19)	120.2
C(3)-C(4)-C(5)	118.5(3)	C(20)-C(19)-H(19)	120.2
C(3)-C(4)-H(4)	120.7	C(19)-C(20)-C(21)	120.0(3)
C(5)-C(4)-H(4)	120.7	C(19)-C(20)-H(20)	120.0

C(21)-C(20)-H(20)	120.0	C(37A)-C(36)-H(36)	101.0
C(20)-C(21)-C(16)	120.7(3)	C(37B)-C(36)-H(36)	122.8
C(20)-C(21)-H(21)	119.7	C(41)-C(40)-C(45)	117.8(3)
C(16)-C(21)-H(21)	119.7	C(41)-C(40)-P(3)	124.7(2)
C(23)-C(22)-C(27)	118.7(2)	C(45)-C(40)-P(3)	117.5(2)
C(23)-C(22)-P(2)	123.6(2)	C(42)-C(41)-C(40)	120.8(3)
C(27)-C(22)-P(2)	117.6(2)	C(42)-C(41)-H(41)	119.6
C(22)-C(23)-C(24)	120.5(3)	C(40)-C(41)-H(41)	119.6
C(22)-C(23)-H(23)	119.7	C(43)-C(42)-C(41)	120.5(3)
C(24)-C(23)-H(23)	119.7	C(43)-C(42)-H(42)	119.8
C(25)-C(24)-C(23)	120.3(3)	C(41)-C(42)-H(42)	119.8
C(25)-C(24)-H(24)	119.9	C(42)-C(43)-C(44)	119.3(3)
C(23)-C(24)-H(24)	119.9	C(42)-C(43)-H(43)	120.4
C(24)-C(25)-C(26)	120.1(3)	C(44)-C(43)-H(43)	120.4
C(24)-C(25)-H(25)	120.0	C(45)-C(44)-C(43)	120.1(3)
C(26)-C(25)-H(25)	120.0	C(45)-C(44)-H(44)	119.9
C(25)-C(26)-C(27)	119.7(3)	C(43)-C(44)-H(44)	119.9
C(25)-C(26)-H(26)	120.1	C(44)-C(45)-C(40)	121.5(3)
C(27)-C(26)-H(26)	120.1	C(44)-C(45)-H(45)	119.2
C(26)-C(27)-C(22)	120.7(3)	C(40)-C(45)-H(45)	119.2
C(26)-C(27)-H(27)	119.6	O(1)-C(46)-Fe(1)	173.3(3)
C(22)-C(27)-H(27)	119.6	O(2)-C(47)-Fe(1)	174.7(3)
C(29)-C(28)-C(33)	118.0(3)	C(35)-C(34A)-C(39A)	116.6(10)
C(29)-C(28)-P(2)	121.3(2)	C(35)-C(34A)-P(3)	120.7(8)
C(33)-C(28)-P(2)	120.6(2)	C(39A)-C(34A)-P(3)	122.6(9)
C(30)-C(29)-C(28)	120.9(3)	C(38A)-C(37A)-C(36)	119.0(5)
C(30)-C(29)-H(29)	119.5	C(38A)-C(37A)-H(37A)	120.5
C(28)-C(29)-H(29)	119.5	C(36)-C(37A)-H(37A)	120.5
C(31)-C(30)-C(29)	119.9(3)	C(37A)-C(38A)-C(39A)	120.5(5)
C(31)-C(30)-H(30)	120.0	C(37A)-C(38A)-H(38A)	119.8
C(29)-C(30)-H(30)	120.0	C(39A)-C(38A)-H(38A)	119.8
C(32)-C(31)-C(30)	119.9(3)	C(38A)-C(39A)-C(34A)	121.1(7)
C(32)-C(31)-H(31)	120.0	C(38A)-C(39A)-H(39A)	119.4
C(30)-C(31)-H(31)	120.0	C(34A)-C(39A)-H(39A)	119.4
C(31)-C(32)-C(33)	120.1(3)	C(39B)-C(34B)-C(35)	118.5(12)
C(31)-C(32)-H(32)	119.9	C(39B)-C(34B)-P(3)	121.0(11)
C(33)-C(32)-H(32)	119.9	C(35)-C(34B)-P(3)	120.4(10)
C(32)-C(33)-C(28)	121.1(3)	C(38B)-C(37B)-C(36)	121.7(5)
C(32)-C(33)-H(33)	119.5	C(38B)-C(37B)-H(37B)	119.1
C(28)-C(33)-H(33)	119.5	C(36)-C(37B)-H(37B)	119.1
C(34A)-C(35)-C(36)	123.5(6)	C(37B)-C(38B)-C(39B)	119.7(6)
C(34A)-C(35)-C(34B)	20.8(5)	C(37B)-C(38B)-C(38B)#1	108.4(6)
C(36)-C(35)-C(34B)	123.1(7)	C(39B)-C(38B)-C(38B)#1	101.9(5)
C(34A)-C(35)-H(35)	113.7	C(37B)-C(38B)-H(38B)	120.1
C(36)-C(35)-H(35)	118.5	C(39B)-C(38B)-H(38B)	120.1
C(34B)-C(35)-H(35)	118.5	C(38B)#1-C(38B)-H(38B)	58.7
C(35)-C(36)-C(37A)	117.6(3)	C(34B)-C(39B)-C(38B)	121.3(9)
C(35)-C(36)-C(37B)	114.4(3)	C(34B)-C(39B)-H(39B)	119.4
C(37A)-C(36)-C(37B)	47.9(3)	C(38B)-C(39B)-H(39B)	119.3
C(35)-C(36)-H(36)	122.8		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[PhBP_3]Fe(CO)_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	21(1)	18(1)	19(1)	-1(1)	4(1)	-3(1)
P(1)	22(1)	17(1)	16(1)	-2(1)	-1(1)	0(1)
P(2)	17(1)	19(1)	17(1)	-1(1)	0(1)	-1(1)
P(3)	23(1)	21(1)	18(1)	1(1)	3(1)	6(1)
O(1)	44(2)	22(1)	82(2)	4(1)	32(1)	0(1)
O(2)	26(1)	48(2)	44(1)	6(1)	-2(1)	-14(1)
B	19(2)	20(2)	18(2)	-2(1)	-2(1)	-2(1)
C(1)	14(1)	18(2)	24(2)	0(1)	-3(1)	8(1)
C(2)	22(2)	25(2)	26(2)	-2(1)	2(1)	2(1)
C(3)	28(2)	25(2)	26(2)	-8(1)	-2(1)	3(1)
C(4)	24(2)	16(2)	39(2)	-2(1)	-4(1)	0(1)
C(5)	25(2)	21(2)	30(2)	2(1)	0(1)	0(1)
C(6)	22(2)	23(2)	20(1)	0(1)	-2(1)	1(1)
C(7)	19(2)	19(2)	20(1)	0(1)	-4(1)	-2(1)
C(8)	21(2)	16(2)	18(1)	-1(1)	3(1)	2(1)
C(9)	38(2)	19(2)	20(1)	-3(1)	-4(1)	-3(1)
C(10)	29(2)	21(2)	17(1)	-2(1)	0(1)	3(1)
C(11)	34(2)	23(2)	30(2)	-2(1)	-5(1)	1(1)
C(12)	47(2)	22(2)	38(2)	2(2)	-4(2)	3(2)
C(13)	49(2)	38(2)	28(2)	5(2)	-9(2)	14(2)
C(14)	38(2)	38(2)	25(2)	-2(2)	-10(1)	4(2)
C(15)	35(2)	24(2)	25(2)	1(1)	-6(1)	1(1)
C(16)	22(2)	19(2)	16(1)	0(1)	-1(1)	2(1)
C(17)	18(2)	31(2)	34(2)	-11(1)	1(1)	1(1)
C(18)	21(2)	33(2)	40(2)	-8(2)	10(1)	-4(1)
C(19)	31(2)	31(2)	21(2)	-4(1)	7(1)	-1(1)
C(20)	32(2)	22(2)	22(2)	-5(1)	0(1)	-3(1)
C(21)	22(2)	17(2)	25(2)	2(1)	3(1)	-2(1)
C(22)	17(1)	19(2)	16(1)	2(1)	-1(1)	3(1)
C(23)	20(2)	23(2)	22(2)	1(1)	-1(1)	-3(1)
C(24)	30(2)	33(2)	25(2)	2(1)	5(1)	-7(1)
C(25)	31(2)	44(2)	17(2)	-3(1)	3(1)	-1(2)
C(26)	33(2)	30(2)	21(2)	-5(1)	-2(1)	-3(1)
C(27)	22(2)	24(2)	23(2)	0(1)	0(1)	-2(1)
C(28)	18(2)	27(2)	15(1)	3(1)	1(1)	-1(1)
C(29)	23(2)	32(2)	25(2)	-5(1)	-1(1)	1(1)
C(30)	25(2)	38(2)	38(2)	-8(2)	1(1)	12(2)
C(31)	18(2)	45(2)	32(2)	-3(2)	-2(1)	8(2)
C(32)	21(2)	38(2)	30(2)	-1(2)	-2(1)	-6(1)
C(33)	24(2)	25(2)	28(2)	-2(1)	1(1)	-2(1)
C(35)	21(2)	28(2)	21(2)	-2(1)	4(1)	0(1)
C(36)	26(2)	44(2)	30(2)	2(2)	2(1)	10(2)
C(40)	25(2)	27(2)	17(1)	5(1)	5(1)	6(1)
C(41)	29(2)	27(2)	24(2)	3(1)	3(1)	3(1)
C(42)	37(2)	37(2)	29(2)	7(2)	-1(2)	9(2)
C(43)	58(2)	29(2)	29(2)	9(2)	13(2)	6(2)
C(44)	49(2)	41(2)	39(2)	13(2)	10(2)	-14(2)
C(45)	29(2)	52(2)	33(2)	15(2)	1(1)	-10(2)
C(46)	30(2)	25(2)	40(2)	-1(2)	17(2)	2(1)
C(47)	33(2)	23(2)	22(2)	-1(1)	-1(1)	-5(2)
C(34A)	16(5)	10(6)	8(3)	-4(4)	-2(3)	0(3)

C(37A)	13(3)	35(4)	26(3)	-8(3)	3(2)	5(3)
C(38A)	31(4)	39(4)	17(3)	2(3)	7(3)	9(3)
C(39A)	23(3)	22(3)	18(3)	-2(2)	-1(2)	9(2)
C(34B)	27(7)	11(6)	26(4)	-2(5)	4(4)	-5(4)
C(37B)	23(4)	35(4)	35(4)	-1(3)	13(3)	15(3)
C(38B)	37(4)	34(4)	23(3)	-4(3)	6(3)	11(3)
C(39B)	25(4)	38(4)	20(3)	1(3)	1(3)	12(3)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[PhBP_3]Fe(CO)_2$.

	x	y	z	U(eq)
H(2)	1023	4989	521	29
H(3)	-162	3844	314	32
H(4)	-1262	3204	1026	32
H(5)	-1090	3719	1962	31
H(6)	131	4848	2176	26
H(7A)	719	6208	2332	23
H(7B)	-201	6465	1754	23
H(8A)	3701	5306	1733	22
H(8B)	2739	5112	2232	22
H(9A)	1320	6563	781	31
H(9B)	2372	5872	694	31
H(11)	1327	9013	1720	36
H(12)	111	9792	1028	43
H(13)	-1523	9237	349	47
H(14)	-1983	7911	387	42
H(15)	-719	7128	1070	34
H(17)	-905	7240	2639	33
H(18)	-1705	7805	3451	37
H(19)	-373	8719	3985	33
H(20)	1781	9069	3706	31
H(21)	2563	8522	2881	26
H(23)	2062	5302	3074	26
H(24)	1179	5416	3970	35
H(25)	1723	6488	4552	37
H(26)	3236	7431	4265	34
H(27)	4123	7319	3373	27
H(29)	5253	4745	2368	32
H(30)	7332	4195	2751	41
H(31)	8950	4946	3309	38
H(32)	8500	6248	3474	36
H(33)	6411	6793	3110	31
H(35)	6074	6222	1578	28
H(36)	7922	5555	1221	40
H(41)	1439	7463	142	32
H(42)	1244	8518	-487	42
H(43)	3012	9430	-476	46
H(44)	5011	9264	157	51
H(45)	5209	8215	782	45
H(37A)	8318	5578	337	29
H(38A)	6915	6348	-302	34
H(39A)	4930	6915	-9	25
H(37B)	7330	4877	305	36
H(38B)	5416	5252	-302	38
H(39B)	3850	6130	20	33